Alma Mater Studiorum - Università di Bologna

DOTTORATO DI RICERCA

FISICA

Ciclo XXI

Settore scientifico disciplinare di afferenza: FIS/02

TITOLO TESI

Effective mapping of spin-1 chains onto integrable fermionic models

Presentata da: dott. Mario Di Dio

Coordinatore Dottorato
Prof. Fabio Ortolani

Relatore
Prof. Giuseppe Morandi

Correlatore
Dr. Cristian Degli Esposti Boschi

Esame finale anno 2009

Contents

List of Figures

List of Tables

Introduction

Dimensionality has a fundamental role in determining the physics of a system. One dimensional models are particularly interesting, since, in a sense, 1-D theories are strongly interacting, because particles cannot avoid themselves in their motion. Furthermore one more feature makes these systems “attractive”: the special symmetry of having just one spatial dimension together with the temporal one, makes them “easier” to address, while preserving and creating new interesting non trivial situations. For example, a number of theories are known to be exactly solvable in one dimension, and quantum field theory methods are extremely powerful and direct.

The study of spin chains has a very long history, going back at least to the investigations of Ernst Ising [1] on the model known with his name and to the solution found by Hans Bethe in 1931 [27] for the spin 1/2 case in one dimension. A very striking feature of spin chains is that their excitation spectrum is completely different, depending on wheter the spin is integer or half-integer. For the spin 1/2 case the Bethe ansatz solution predicts gapless excitations. Lieb, Shultz and Mattis (1961) [2] proved that for an antiferromagnetic spin 1/2 Heisenberg chain with an even number L of sites[1], at least one excited state exists which is separated from the ground state by an energy $O(L^{-1})$. The one-magnon spectrum was calculated by des Cloizeaux and Pearson [28] who showed that the chain is gapless and the ground state is almost long range ordered. It was only in 1983 that Haldane [33], [34] suggested that antiferromagnetic integer spin chains have a disordered ground state and a finite gap in the excitation spectrum. From the assumption that the system retains a short-range antiferromagnetic order, despite the

[1]This result was later generalized by Affleck and Lieb [3] for generic half-integer spin.

strong quantum fluctuations, he was able to map, in the low energy and large correlation lenght limit, the lattice model onto the $O(3)$ Non Linear Sigma model (NLσM) with a topological term.

In the 1970-s low dimensional physics stopped being just a theoretical "toy", since it became clear that the theoretical models were actually very useful in the description of real materials. Later on, in the 1980-s, the discovery of the Quantum Hall Effect and high temperature superconductivity, among others, brought increasing attention to low dimensional physics. In recent years, zero dimensional (*quantum dots*) and one dimensional (*quantum wires*) systems have been implemented in laboratories as well.

Low dimensional systems, and quantum spin chains, in particular, are of great interest in Quantum Information Theory. Since the unit of Quantum information is the *qubit*, i.e. the information described by a state vector of a two level quantum system, quantum spin chains arise as natural candidates for the implementation of quantum devices.

The thesis is organized as follows. In the first chapter we review the fundamental properties of spin 1/2 Heisenberg chains with nearest neighbor interactions. Following the seminal paper by Lieb, Shultz and Mattis (1961) [2] we describe the general method to diagonalize hamiltonians quadratic in Fermi operators, and derive the general expression for the spin-spin correlations. We specialize then to the XY model in a magnetic field: we give a detailed account for the diagonalization of the model and we write down its spin-spin correlation functions [11]. We finally discuss the duality properties of the model.

Chapter 2 is devoted to the study of spin-1 Heisenberg chains. We will first review the semiclassical limit of the quantum Heisenberg spin chain using the Holstein-Primakoff approach to spin wave theory [30], [31], showing that, while the ferromagnet has a quadratic dispersion relation and thus it is not possible to find a corresponding Lorentz invariant field theory, the antiferromagnetic chain instead has a relativistic (linear) dispersion relation and thus can have a corresponding Lorentz invariant field theory. We will then see [30], [32], [34] that the large spin, low energy, continuum limit of the antiferromagnetic quantum chain maps aproximately onto the $O(3)$ non linear σ model with a topological term: it is this term that makes the behavior of the integer and half-integer spin chain completely different. We will briefly discuss the nonlocal string order parameter proposed by den Nijs and Rommelse in 1989 [38] to detect the hidden order of the so called *Haldane phase*, and show how the non vanishing of the string order parameter is actually a sign of the spontaneous breaking of a hidden $Z_2 \times Z_2$ symmetry [41], [40]. Finally we will work out in detail the exactly solvable spin 1 model with a spin gap and string order provided by Affleck, Kennedy, Lieb and Tasaki in 1987 [42], [43].

In Chapter 3 we derive the dominant contribution to the large-distance decay laws of correlation functions towards their asymptotic limits for a spin chain model (the so called λ-D model) that exhibits both Haldane and Néel phases in its ground state phase diagram. The analytic results are obtained by means of an approximate mapping between a spin-1 anisotropic Hamiltonian onto a fermionic model of noninteracting Bogoliubov quasiparticles related in turn (via Jordan-Wigner transformation) to the XY spin-1/2 chain in a transverse field. This approach allows us to express the spin-1 string operators in terms of fermionic operators so that the dominant contribution to the string correlators at large distances can be computed using the technique of Toeplitz determinants. As expected, we find long-range string order both in the longitudinal and in the transverse channel in the Haldane phase, while in the Néel phase only the longitudinal order survives. In this way, the long-range string order can be explicitly related to the components of the magnetization of the XY model. Moreover, apart from the critical line, where the decay is algebraic, we find that in the gapped phases the decay is governed by an exponential tail multiplied by power-law factors. As regards the usual two points correlation functions, we show that the longitudinal one behaves in a "dual" fashion with respect to the transverse string correlator, namely both the asymptotic values and the decay laws exchange when the transition line is crossed. For the transverse spin-spin correlator, we always find a finite characteristic length which is an unexpected feature at the critical point. The results of this analysis prove some conjectures put forward in the past. The goodness of the approximation and the analytical predictions are checked versus density-matrix renormalization group calculations.

In the fourth Chapter we discuss the entanglement properties of the λ-

D model. We briefly introduce the idea of separability of mixed states and the Peres-Horodecki criterion; we study the partial transpose of the two-site density matrix of the system, obtaining an analytic expression for the so called *negativity* of the λ-D model. Following the same approach used in the previous chapter we get an expression of the negativity in terms of the correlators previously calculated.

We dedicate a chapter to the Conclusions, where we summarize our main original results discussed in Chapter 3 and Chapter 4.

Finally in Appendix A we review the main results on Toeplitz forms and the asymptotics of Toeplitz determinants, and in Appendix B we present the detailed calculation of the transverse spin-spin correlator of the λ-D model, because it cannot be related directly to other spin-1/2 correlators calculated previously in the literature.

Chapter 1

Anisotropic spin $1/2$ Heisenberg chains

In this section we will consider one dimensional spin 1/2 anisotropic Heisenberg chains in a magnetic field. Following the paper by Lieb, Schultz and Mattis(1961) [2] we will outline the general method to diagonalize Heisenberg hamiltonians, and we will then specialize to the XY model in a transverse magnetic field.

1.1 Outline of the method

Let's consider the most general spin 1/2 Heisenberg hamiltonian with nearest-neighbours interactions in a magnetic field [4]

$$\mathcal{H} = \sum_l \left(J_x \sigma_l^x \sigma_{l+1}^x + J_y \sigma_l^y \sigma_{l+1}^y + J_z \sigma_l^z \sigma_{l+1}^z \right) + h \sum_l \sigma_l^z \tag{1.1}$$

where σ_l^α are the Pauli matrices acting on site l and the J_α are the anisotropies along the direction α. Let's introduce the operators

$$\sigma_l^\pm = \frac{\sigma_l^x \pm i\sigma_l^y}{2} \tag{1.2}$$

in terms of which we can rewrite the hamiltonian as

$$\mathcal{H} = \sum_l \big[(J_x - J_y) \left(\sigma_l^+ \sigma_{l+1}^+ + \sigma_l^- \sigma_{l+1}^- \right) + (J_x + J_y) \left(\sigma_l^+ \sigma_{l+1}^- + \sigma_l^- \sigma_{l+1}^+ \right)$$

$$+J_z\sigma_l^z\sigma_{l+1}^z\big] + h\sum_l \sigma_l^z \tag{1.3}$$

We now introduce the Jordan-Wigner transformations [5]

$$\sigma_l^+ = c_l^\dagger \exp\left[i\pi\sum_{k<l} c_k^\dagger c_k\right] \qquad\qquad \sigma_l^- = \exp\left[-i\pi\sum_{k<l} c_k^\dagger c_k\right] c_l$$

$$\sigma_l^z = 2c_l^\dagger c_l - 1 \tag{1.4}$$

where c_l, $c_l^\dagger$ are fermionic operators. It is straightforward to verify that [2]

$$\exp\left[i\pi c_k^\dagger c_k\right] = \exp\left[-i\pi c_k^\dagger c_k\right]$$

and

$$c_l^\dagger c_{l+1} = \sigma_l^+\sigma_{l+1}^- \qquad\qquad c_l^\dagger c_{l+1}^\dagger = \sigma_l^+\sigma_{l+1}^+ \tag{1.5}$$

The hamiltonian becomes then

$$\mathcal{H} = \sum_l \Big[(J_x - J_y)\left(c_l^\dagger c_{l+1}^\dagger + c_l c_{l+1}\right) + (J_x + J_y)\left(c_l^\dagger c_{l+1} + c_l c_{l+1}^\dagger\right)$$

$$+ J_z\left(2n_l - 1\right)\left(2n_{l+1} - 1\right)\Big] + h\sum_l \left(2n_l - 1\right) \tag{1.6}$$

if the hamiltonian has open boundary conditions. In case of cyclic boundary conditions

$$\mathcal{H}_{cyclic} = \mathcal{H} - \mathcal{H}_b$$

where

$$\mathcal{H}_b = \left[(J_x - J_y)\left(c_N^\dagger c_1^\dagger + h.c.\right) + (J_x + J_y)\left(c_N^\dagger c_1 + h.c.\right)\right]$$

$$\cdot\left(\exp\left(i\pi\sum_{k=1}^{N} c_k^\dagger c_k\right) + 1\right)$$

For large systems it is possible to neglect the additional term $\mathcal{H}_b$.

1.1.1 Exact diagonalization of a general quadratic form in fermionic operators

We will now show [2] that every hamiltonian quadratic in fermion operators can be exactly diagonalized. Let

$$H = \sum_{m,n} \left[c_m^\dagger A_{m,n} c_n + \frac{1}{2} \left(c_m^\dagger B_{m,n} c_n^\dagger + h.c. \right) \right] \tag{1.7}$$

be a general hermitean quadratic form in Fermi operators. The hermiticity of H implies that A is a hermitean matrix, and the anticommutation relations between fermion operator require B to be antisymmetric. With no loss of generality, we will assume A and B to be real matrices.

We try to find a canonical transformation

$$\eta_p^\dagger = \sum_m \left(f_{pm} c_m^\dagger + g_{pm} c_m \right)$$

$$\eta_p = \sum_m \left(f_{p,m} c_m + g_{p,m} c_m^\dagger \right) \tag{1.8}$$

such that

$$H = \sum_p \Lambda_p \eta_p^\dagger \eta_p + const.$$

This is possible if

$$[\eta_p, H] - \Lambda_p \eta_p = 0 \tag{1.9}$$

Inserting (1.8) into (1.9), setting then the coefficients of every operator equal to zero, we get the set of equations

$$\Lambda_p f_{p,m} = \sum_n \left(f_{p,n} A_{n,m} - g_{p,n} B_{n,m} \right)$$

$$\Lambda_p g_{p,m} = \sum_n \left(f_{p,n} B_{n,m} - g_{p,n} A_{n,m} \right) \tag{1.10}$$

that become

$$\Lambda_p \phi_p = (A - B)\, \psi_p$$

$$\Lambda_p \psi_p = (A + B)\, \phi_p \tag{1.11}$$

where we have defined

$$\phi_p = f_{p,m} + g_{p,m} \qquad\qquad \psi_p = f_{p,m} - g_{p,m} \tag{1.12}$$

From the last set of equations (1.11) we can get either [2]

$$\phi_p\, (A - B)\, (A + B) = \Lambda_p^2 \phi_p \tag{1.13}$$

or

$$\psi_p\, (A + B)\, (A - B) = \Lambda_p^2 \psi_p \tag{1.14}$$

For $\Lambda_p \neq 0$ either (1.13) or (1.14) can be solved for ϕ_p or ψ_p and the other vector is found from (1.11). If $\Lambda_p = 0$ the vectors ϕ_p, ψ_p are obtained from (1.11), their relative sign being arbitrary. Changing the sign of ψ_p, but not that of ϕ_p results in exchanging the role of $f_{p,m}$ and $g_{p,m}$, thus exchanging the definition of occupied and unoccupied zero energy modes.

Noting that $(A + B)^T = (A - B)$, we immediately find that both $(A - B)\,(A + B)$ and $(A + B)\,(A - B)$ are symmetric and at least semi definite positive; it then follows that all the Λ_p are real, and it is possible to choose ϕ_p and ψ_p to be real as well as orthonormal, i.e.

$$\sum_m \left(f_{p,m} f_{p',m} + g_{p,m} g_{p',m} \right) = \delta_{p,p'} \tag{1.15}$$

$$\sum_m \left(f_{p,m} g_{p',m} - f_{p',m} g_{p,m} \right) = 0 \tag{1.16}$$

Finally, from the invariance of trH under canonical transformations we find the constant to be [2]

$$const. = \frac{1}{2} \left(\sum_m A_{m,m} - \sum_p \Lambda_p \right) \tag{1.17}$$

1.1.2 General expression for the correlation functions

Correlation functions are very useful quantities to distinguish the various regions of the phase diagrams of statistical models.

We will calculate general expressions for the correlation functions of models whose hamiltonians are quadratic in Fermi operators; we define the correlators as

$$\rho^{\alpha}_{j,l} = \langle \sigma^{\alpha}_j \sigma^{\alpha}_l \rangle \tag{1.18}$$

where $\alpha = x, y, z$. The first step is to express the correlation functions in terms of fermionic operators; we get

$$\rho^{x}_{j,l} = \langle \sigma^{x}_j \sigma^{x}_l \rangle = \langle \left(\sigma^+_j + \sigma^-_j\right) \left(\sigma^+_l + \sigma^-_l\right) \rangle$$

$$= \langle \left(c^\dagger_j + c_j\right) \exp\left(i\pi \sum_{k<j} c^\dagger_k c_k\right) \exp\left(i\pi \sum_{k<l} c^\dagger_k c_k\right) \left(c^\dagger_l + c_l\right) \rangle$$

Since

$$\exp\left(i\pi \sum_{k<l} c^\dagger_k c_k\right) = \prod_{k<l} \left(1 - 2c^\dagger_k c_k\right)$$

and

$$\left(1 - 2c^\dagger_k c_k\right) = \left(c^\dagger_k + c_k\right) \left(c^\dagger_k - c_k\right)$$

we obtain for the correlator [2]

$$\rho^{x}_{j,l} = \langle B_j A_{j+1} B_{j+1} \cdots A_{l-1} B_{l-1} A_l \rangle \tag{1.19}$$

where we have defined

$$A_k = c^\dagger_k + c_k \qquad\qquad B_k = c^\dagger_k - c_k \tag{1.20}$$

Using Wick's theorem, Caianiello and Fubini [6] have shown that vacuum expection values of anticommuting operators, like (1.19), can be expressed as pfaffians, i.e.

$$\rho^{x}_{j,l} = pf \left| \begin{array}{cccccccc} S_{j,j+1} & S_{j,j+2} & \cdots & S_{j,l-1} & G_{j,j+1} & \cdots & \cdots & G_{j,l} \\ & S_{j+1,j+2} & \cdots & S_{j+1,l-1} & G_{j+1,j+1} & \cdots & \cdots & G_{j+1,l} \\ & & \ddots & \vdots & \vdots & \cdots & \cdots & \vdots \\ & & & S_{l-2,l-1} & G_{l-2,j+1} & \cdots & \cdots & G_{l-2,l} \\ & & & & G_{l-1,j+1} & \cdots & \cdots & G_{l-1,l} \\ & & & & & Q_{j+1,j+2} & \cdots & Q_{j+1,l} \\ & & & & & & \ddots & \vdots \\ & & & & & & & Q_{l-1,l} \end{array} \right| \tag{1.21}$$

with

$$S_{j,l} = \langle B_j B_l \rangle \qquad Q_{j,l} = \langle A_j A_l \rangle \qquad G_{j,l} = \langle B_j A_l \rangle \tag{1.22}$$

For a generic $2n \times 2n$ skew symmetric matrix $M = \{m_{i,j}\}$ the pfaffian [15] is a polynomial of degree n, defined as

$$pf(M) = \frac{1}{2^n n!} \sum_{\sigma \in S_{2n}} \operatorname{sgn}(\sigma) \prod_{i=1}^{n} m_{\sigma(2i-1),\sigma(2i)} \tag{1.23}$$

where S_{2n} is the symmetric group and $\operatorname{sgn}(\sigma)$ is the sign of σ. A remarkable property of the pfaffian that symplifies its calculation is that

$$pf(M) = \sqrt{det(M)} \tag{1.24}$$

The calculation of the pfaffian (1.21) greatly simplifies since a certain number of contractions vanishes

$$\langle A_j A_l \rangle = \sum_k \phi_{k,j} \phi_{k,l} = \delta_{j,l} \tag{1.25}$$

$$\langle B_j B_l \rangle = -\sum_k \psi_{k,j} \psi_{k,l} = -\delta_{j,l} \tag{1.26}$$

$$\langle B_j A_l \rangle = -\langle A_l B_j \rangle = -\sum_k \psi_{k,j} \phi_{k,l} = \delta_{j,l} \tag{1.27}$$

The correlation function reduces then to [2]

$$\rho^x_{j,l} = det \begin{vmatrix} G_{j,j+1} & \cdots & G_{j,l} \\ \vdots & \ddots & \vdots \\ G_{l-1,j+1} & \cdots & G_{l-1,l} \end{vmatrix} \tag{1.28}$$

Furthermore, in the cyclic problem, the hamiltonian is translation invariant, so that $G_{j,l} = G_{j-l}$, i.e. they depend only on the relative distance.

In the same way we get [2]

$$\rho^y_{j,l} = (-1)^{l-j} \langle A_j B_{j+1} A_{j+1} \cdots B_{l-1} A_{l-1} B_l \rangle \tag{1.29}$$

$$= (-1)^{l-j} \, det \begin{vmatrix} -G_{j+1,j} & \cdots & -G_{j+1,l-1} \\ \vdots & \ddots & \vdots \\ -G_{l,j} & \cdots & -G_{l,l-1} \end{vmatrix} = det \begin{vmatrix} G_{j+1,j} & \cdots & G_{j+1,l-1} \\ \vdots & \ddots & \vdots \\ G_{l,j} & \cdots & G_{l,l-1} \end{vmatrix}$$

The calculation of the transverse correlation function $\rho^z_{j,l}$ is quite straightforward; in fact [2]

$$\rho^z_{j,l} = \langle \sigma^z_j \sigma^z_l \rangle = \langle (2n_j - 1)\,(2n_l - 1) \rangle = \langle A_j B_j A_l B_l \rangle$$

$$= \langle A_j B_j \rangle \langle A_l B_l \rangle + \langle A_j B_l \rangle \langle B_j A_l \rangle = G_{j,j} G_{l,l} - G_{l,j} G_{j,l} \qquad (1.30)$$

1.2 The spin $1/2$ XY model in a magnetic field

The spin 1/2 XY spin chain is one of the easiest non trivial quantum integrable models. It describes a one dimensional lattice system, with each site occupied by a spin 1/2 degree of freedom, that interacts with its nearest neighbors, the interectation being restricted to x and y directions; we will study the effect of an external transverse magnetic field, interacting with the z components of spins. The hamiltonian of the model is usually written as[1]

$$\mathcal{H}_{XY} = \sum_{j=1}^{N} \left[\left(\frac{1+\gamma}{2} \right) \sigma^x_j \sigma^x_{j+1} + \left(\frac{1-\gamma}{2} \right) \sigma^y_j \sigma^y_{j+1} \right] - h \sum_{j=1}^{N} \sigma^z_j \qquad (1.31)$$

where γ is the anisotropy parameter and h is the external magnetic field, and periodic boundary conditions are imposed, i.e $\sigma^\alpha_1 = \sigma^\alpha_N$.

It is possible to diagonalize the hamiltonian following the steps described above: first we use a Jordan-Wigner transformation, mapping the spin degrees of freedom onto spinless fermions, then a Bogolubov transformation defines Bogolubov quasi-particles, in terms of which the model reduces to lattice free fermions. Despite its symplicity, the model is far from trivial: the quasi-particles are non local in terms of the original degrees of freedom, so that every quantity (i.e. correlation functions and so on) of the original model we wish to calculate has a non trivial expression in terms of free fermions.

[1] We put in (1.1) $J_x - J_y = \gamma$, $J_x + J_y = 1$ and $J_z = 0$

1.2.1 Diagonalization of the model

We will now work out in detail all the steps neccessary to diagonalize the model (1.31). Define the Jordan-Wigner transformation

$$\sigma_j^+ = c_j^\dagger \exp\left[i\pi \sum_{l<j} c_l^\dagger c_l\right] \qquad\qquad \sigma_j^- = \exp\left[-i\pi \sum_{l<j} c_l^\dagger c_l\right] c_j$$

$$\sigma_j^z = 2c_j^\dagger c_j - 1 \tag{1.32}$$

where c_j, $c_j^\dagger$ are fermionic operators. The hamiltonian (1.31) in terms of these spinless fermions becomes

$$\mathcal{H}_{XY} = \sum_{j=1}^{N} \left(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j + \gamma c_j^\dagger c_{j+1}^\dagger + \gamma c_{j+1} c_j - 2h c_j^\dagger c_j + h\right) \tag{1.33}$$

In Fourier space ($c_k = \sum_j c_j e^{-ikj}$) the hamiltonian becomes

$$\mathcal{H}_{XY} = \sum_{j=1}^{N} \left[2\left(\cos k - h\right) c_k^\dagger c_k + i\gamma \sin k \left(c_k^\dagger c_{-k}^\dagger + c_k c_{-k}\right) + h\right] \tag{1.34}$$

This hamiltonian can be diagonalized by the Bogolubov transformation

$$\eta_k = \cos\frac{\theta_k}{2} c_k + i \sin\frac{\theta_k}{2} c_{-k}^\dagger \tag{1.35}$$

where θ_k is defined by

$$e^{i\theta_k} = \frac{\cos k - h + i\gamma \sin k}{\Lambda_k} \tag{1.36}$$

and the quasi-particle spectrum

$$\Lambda_k = \sqrt{\left(\cos k - h\right)^2 + \gamma^2 \sin^2 k} \tag{1.37}$$

We finally get the hamiltonian in diagonal form

$$\mathcal{H}_{XY} = \sum_k \Lambda_k \left(\eta_k^\dagger \eta_k - \frac{1}{2}\right) \tag{1.38}$$

A system is critical when its spectrum is gapless; when it is critical, a system undergoes a quantum phase transition [7], a zero temperature analog of classical phase transitions. Furthermore quantum phase transitions are

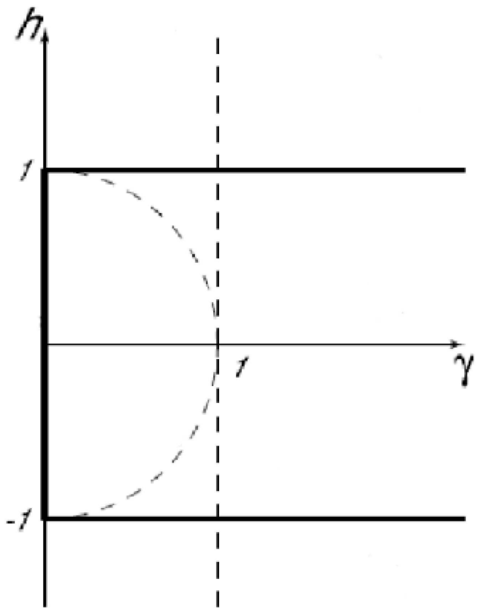

Figure 1.1: Phase diagram of the XY model

characterized by singularities in thermodynamic quantities and a algebraic behavior of the correlation functions.

From (1.37) we see that the XY model is critical when $h = \pm 1$, and $\gamma = 0$ and $|h| < 1$. It can be noticed from Figure 1.1 that the model is symmetric under the transformations $h \to -h$ and $\gamma \to -\gamma$; the critical lines are depicted with bold lines and separate three non critical regions, the dotted lines show the very special lines $\gamma = 1$ when the model reduces to the Ising model in a transverse field, and $h^2 + \gamma^2 = 1$ where the ground state can be written as a product of single site wave functions [14]

$$|\Psi_\pm\rangle = \prod_j \left[\cos\theta |\uparrow_j\rangle \pm \sin\theta |\downarrow_j\rangle\right] \tag{1.39}$$

where $\cos^2\theta = (1-\gamma)\,/\,(1+\gamma)$ and the product runs over the lattice sites.

1.2.2 Correlators of the model

The correlation functions of the XY model have been found in the seventies by B.McCoy and coauthors [9], [10], [11] in various regimes (in a time dependent magnetic field, non zero temperature, and so on). In this subsection we will give the detailed results of the correlation functions of the model in a transverse field at zero temperature (without giving the details of the calculations[2]).

In terms of the Bogolubov quasi particles, the ground state is defined as

$$\eta_k|0\rangle = 0 \qquad \forall k \tag{1.40}$$

the usual vacuum for free fermions. It is straightforward to find that the correlators are

$$\langle 0|\eta_k \eta_{k'}|0\rangle = \langle 0|\eta_k^\dagger \eta_{k'}^\dagger|0\rangle = \langle 0|\eta_k^\dagger \eta_{k'}|0\rangle = 0$$

$$\langle 0|\eta_k \eta_{k'}^\dagger|0\rangle = \delta_{k,k'} \tag{1.41}$$

The calculation becomes more difficult when we express the ground state of the model in terms of physical particles. We can invert the Bogolubov transformation(1.35)

$$c_k = \cos\frac{\theta_k}{2}\eta_k - i\sin\frac{\theta_k}{2}\eta_{-k}^\dagger \tag{1.42}$$

to calculate the correlators in terms of physical fermions

$$\langle 0|c_k c_{k'}|0\rangle = \langle 0|\left(\cos\frac{\theta_k}{2}\eta_k - i\sin\frac{\theta_k}{2}\eta_{-k}^\dagger\right)\left(\cos\frac{\theta_{k'}}{2}\eta_{k'} - i\sin\frac{\theta_{k'}}{2}\eta_{-k'}^\dagger\right)|0\rangle$$

$$= -i\sin\frac{\theta_{k'}}{2}\cos\frac{\theta_k}{2}\delta_{k,-k'} \tag{1.43}$$

$$\langle 0|c_k^\dagger c_{k'}^\dagger|0\rangle = \langle 0|\left(\cos\frac{\theta_k}{2}\eta_k^\dagger + i\sin\frac{\theta_k}{2}\eta_{-k}\right)\left(\cos\frac{\theta_{k'}}{2}\eta_{k'}^\dagger + i\sin\frac{\theta_{k'}}{2}\eta_{-k'}\right)|0\rangle$$

$$= i\sin\frac{\theta_k}{2}\cos\frac{\theta_{k'}}{2}\delta_{-k,k'} \tag{1.44}$$

$$\langle 0|c_k^\dagger c_{k'}|0\rangle = \langle 0|\left(\cos\frac{\theta_k}{2}\eta_k^\dagger + i\sin\frac{\theta_k}{2}\eta_{-k}\right)\left(\cos\frac{\theta_{k'}}{2}\eta_{k'} - i\sin\frac{\theta_{k'}}{2}\eta_{-k'}^\dagger\right)|0\rangle$$

[2]See [9], [10], [11], [12], [13]

$$= \sin\frac{\theta_k}{2}\sin\frac{\theta_{k'}}{2}\delta_{k,k'} \tag{1.45}$$

$$\langle 0|c_k c^\dagger_{k'}|0\rangle = \langle 0|\left(\cos\frac{\theta_k}{2}\eta_k - i\sin\frac{\theta_k}{2}\eta^\dagger_{-k}\right)\left(\cos\frac{\theta_{k'}}{2}\eta^\dagger_{k'} + i\sin\frac{\theta_{k'}}{2}\eta_{-k'}\right)|0\rangle$$

$$= \cos\frac{\theta_k}{2}\cos\frac{\theta_{k'}}{2}\delta_{k,k'} \tag{1.46}$$

The two point fermionic correlators can now be obtained by Fourier transform. In the thermodynamic limit they become

$$F_{j,l} = i\langle 0|c_j c_l|0\rangle = -i\langle 0|c^\dagger_j c^\dagger_l|0\rangle = \frac{1}{2\pi}\int_0^{2\pi} dk\frac{\sin\theta_k}{2}e^{ik(j-l)} \tag{1.47}$$

$$H_{j,l} = \langle 0|c_j c^\dagger_l|0\rangle = \frac{1}{2\pi}\int_0^{2\pi} dk\frac{1+\cos\theta_k}{2}e^{ik(j-l)} \tag{1.48}$$

We can now calculate the spin-spin correlation functions of the model. Let's recall their expressions (1.19), (1.29), (1.30)

$$\rho^x_{j,l} = det\begin{vmatrix} G_{j,j+1} & \cdots & G_{j,l} \\ \vdots & \ddots & \vdots \\ G_{l-1,j+1} & \cdots & G_{l-1,l}\end{vmatrix} \tag{1.49}$$

$$\rho^y_{j,l} = det\begin{vmatrix} G_{j+1,j} & \cdots & G_{j+1,l-1} \\ \vdots & \ddots & \vdots \\ G_{l,j} & \cdots & G_{l,l-1}\end{vmatrix} \tag{1.50}$$

$$\rho^z_{j,l} = G_{j,j}G_{l,l} - G_{j,l}G_{l,j} \tag{1.51}$$

where

$$G_{j,l} = \langle 0|B_j A_l|0\rangle = \langle 0|\left(c^\dagger_j - c_j\right)\left(c^\dagger_l + c_l\right)|0\rangle = \frac{i}{2\pi}\int_0^{2\pi} dk\sin\theta_k e^{ik(j-l)}$$

$$+\frac{1}{2\pi}\int_0^{2\pi} dk\frac{1-\cos\theta_k}{2}e^{ik(j-l)} - \frac{1}{2\pi}\int_0^{2\pi} dk\frac{1+\cos\theta_k}{2}e^{ik(j-l)}$$

$$= -\frac{1}{2\pi}\int_0^{2\pi} dk\left(\cos\theta_k - i\sin\theta_k\right)e^{ik(j-l)}$$

$$= -\frac{1}{2\pi}\int_0^{2\pi} dk \frac{\cos k - h - i\gamma \sin k}{\sqrt{(\cos k - h)^2 + \gamma^2 \sin^2 k}} e^{ik(j-l)} = \frac{1}{2\pi}\int_0^{2\pi} g\left(e^{ik}\right) dk \quad (1.52)$$

Matrices like (1.49), (1.50) are known as Toeplitz matrices[3] and a vast mathematical literature has been devoted to the study of the asymptotic behavior of their determinants. T.T.Wu, B.McCoy and coauthors [8], [9], [10], [11] were among the first to develop the theory of Toeplitz determinants in connection to physical systems. The asymptotic properties of Toeplitz determinants are determined by the analytic properties of the function $g\left(e^{ik}\right)$ the so called *symbol* or *generating function* of the Toeplitz determinant. In this section we will summarize the results obtained by McCoy and coauthors without giving the details of the calculation.

Let's start with $\rho^x_{j,l}$. The generating function is [11]

$$g_x\left(e^{ik}\right) = -\left[\frac{\left(1-\lambda_1^{-1}e^{ik}\right)\left(1-\lambda_2^{-1}e^{ik}\right)}{\left(1-\lambda_1^{-1}e^{-ik}\right)\left(1-\lambda_2^{-1}e^{-ik}\right)}\right]^{1/2} \quad (1.53)$$

where

$$\lambda_{1,2} = \frac{h \pm \sqrt{h^2+\gamma^2-1}}{1-\gamma} \quad (1.54)$$

We will distinguish the three cases $h < 1$, $h > 1$ and $h = 1$ [11].

- $h < 1$. The symbol never vanishes on the unit circle $g\left(e^{ik}\right) \neq 0$ and has winding number zero $\mathrm{Ind}\left[g\left(e^{ik}\right)\right] = 0$, thus Szegö strong limit theorem [16] can be used. When $h^2 > 1-\gamma^2$ the asymptotic behavior is

$$\rho^x = (-1)^R \frac{2\left[\gamma^2\left(1-\gamma^2\right)\right]^{1/4}}{1+\gamma}\left[1 + \frac{1}{2\pi\left(\lambda_2-\lambda_2^{-1}\right)^2}\frac{\lambda_2^{-2R}}{R^2}\right] \quad (1.55)$$

while for $h^2 < 1-\gamma^2$

$$\rho^x = (-1)^R \frac{2\left[\gamma^2\left(1-\gamma^2\right)\right]^{1/4}}{1+\gamma}\left\{1 + \frac{\alpha^{2R}}{\pi R^2}\Re\left[e^{i\psi}\left(\alpha^{-1}e^{-i\psi} - \alpha e^{i\psi}\right)^{-2}\right]\right\} \quad (1.56)$$

where

$$\alpha = \sqrt{\frac{1-\gamma}{1+\gamma}} \qquad \psi = \arctan\left[\frac{\sqrt{1-\gamma^2-h^2}}{h}\right] \quad (1.57)$$

[3] See Appendix A for a brief review on Toeplitz forms and the asymptotics of Toeplitz determinants

- $h > 1$. The symbol never vanishes on the unit circle, but its winding number is 1. The asymptotic behavior of the correlator is then

$$\rho^x = (-1)^R \frac{\lambda_2^R}{\pi^{1/2} R^{1/2}} \left[\frac{\left(1-\lambda_1^{-2}\right)\left(1-\lambda_1^{-1}\lambda_2^{-1}\right)^2}{\left(1-\lambda_2^2\right)} \right]^{1/4} \tag{1.58}$$

- $h = 1$. The generating function vanishes at $k = 0$, and Fisher-Hartwig conjecture [18] must be used.

$$\rho^x = (-1)^R \frac{1}{(\gamma R)^{1/4}} \frac{2\gamma e^{1/4} 2^{1/12} A^{-3}}{1+\gamma} \tag{1.59}$$

where $A = 1.282427130$ is Glaisher's constant [19].

Let's now consider ρ^y; the generating function can be written as

$$g_y\left(e^{ik}\right) = -e^{-2ik} \left[\frac{\left(1-\lambda_1^{-1}e^{ik}\right)\left(1-\lambda_2^{-1}e^{ik}\right)}{\left(1-\lambda_1^{-1}e^{-ik}\right)\left(1-\lambda_2^{-1}e^{-ik}\right)} \right]^{1/2} \tag{1.60}$$

The three regions $h < 1$, $h > 1$ and $h = 1$ are obtained again [11].

- $h < 1$. We have $\mathrm{Ind}\left[g_y\left(e^{ik}\right)\right] = -2$, and thus Szegö theorem [16] can be used "shifting" the determinant. If $h^2 > 1 - \gamma^2$

$$\rho^y = -(-1)^R \frac{\lambda_2^{-2R}}{\pi R^3} \frac{2\left[\gamma^2\left(1-h^2\right)\right]^{1/4}}{1+\gamma}$$

$$\cdot \left[\left(1-\lambda_2^{-2}\right)\left(1-\lambda_1^{-1}\lambda_2\right)\left(1-\lambda_1^{-1}\lambda_2^{-1}\right)\right]^{-1/2} \tag{1.61}$$

otherwise, when $h^2 < 1 - \gamma^2$

$$\rho^y = -(-1)^R \frac{\alpha^{2R}}{\pi R} \frac{2\left[\gamma^2\left(1-h^2\right)\right]^{1/4}}{1+\gamma}$$

$$\cdot \left[\left(1-\lambda_2^{-2}\right)\left(1-\lambda_1^{-1}\lambda_2\right)\left(1-\lambda_1^{-1}\lambda_2^{-1}\right)\right]^{-1} \sin^2\psi \tag{1.62}$$

- $h > 1$. In this case $\mathrm{Ind}\left[g_y\left(e^{ik}\right)\right] = -1$, and

$$\rho^y = -(-1)^R \frac{\lambda_2^R}{2\pi^{1/2} R^{3/2}} \left[\frac{\left(1-\lambda_2^2\right)^3\left(1-\lambda_1^{-2}\right)}{\left(1-\lambda_1^{-1}\lambda_2^{-1}\right)^2} \right]^{1/4} \left(1-\lambda_1^{-1}\lambda_2^{-1}\right)^{-1} \tag{1.63}$$

- $h = 1$. The generating function vanishes on the unit circle, and Fisher-Hartwig conjecture [18] must be used.

$$\rho^x = (-1)^R \frac{1}{(\gamma R)^{9/4}} \gamma (1+\gamma) \frac{e^{1/4} 2^{1/12} A^{-3}}{8} \tag{1.64}$$

It is interesting to notice that at the special point $h^2 = 1 - \gamma^2$ both correlators ρ^x and ρ^y can be calculated exactly, giving the results

$$\rho^x = (-1)^R \frac{2\gamma}{1+\gamma} \qquad\qquad \rho^y = 0 \tag{1.65}$$

Let's finally turn our attention to ρ^z; the calculation is easier than the previous correlators since we need just to evaluate the integral G_R [11].

- $h < 1$ and $h^2 > 1 - \gamma^2$

$$\rho^z = m_z^2 - \frac{\lambda_2^{-2R}}{2\pi R^2} \tag{1.66}$$

- $h < 1$ and $h^2 < 1 - \gamma^2$

$$\rho^z = m_z^2 - \frac{4\alpha^{2R}}{\pi R^2} \Re \left\{ e^{i\psi(R+1)} \left[\frac{1 - e^{2i\psi}}{1 - \alpha^2 e^{-2i\psi}} \right]^{1/2} \right\}$$

$$\cdot \Re \left\{ e^{i\psi(R-1)} \left[\frac{1 - \alpha^2 e^{-2i\psi}}{1 - e^{2i\psi}} \right]^{1/2} \right\} \tag{1.67}$$

- $h > 1$

$$\rho^z = m_z^2 - \frac{\lambda_2^{2R}}{2\pi R^2} \tag{1.68}$$

- $h = 1$ and $\gamma \neq 0$

$$\rho^z = m_z^2 - \frac{1}{2\pi R^2} \tag{1.69}$$

where the magnetization is

$$m_z = -\frac{1}{\pi} \int_0^\pi dk \frac{\cos k - h}{\sqrt{(\cos k - h)^2 + \gamma^2 \sin^2 k}} \tag{1.70}$$

Finally when $h^2 = 1 - \gamma^2$, we obtain the exact result $\rho^z = m_z^2$

It is very interesting to notice the presence of an incommensurate phase, the region of parameter space defined by $h^2 + \gamma^2 < 1$, i.e. when the two roots $\lambda_{1,2}$ are complex, which gives rise to oscillating correlation functions (1.56), (1.62), (1.67) with wave number ψ.

1.2.3 Self duality of the XY model

The concept of duality stems from the work of Kramers and Wannier (1941) [23] on the two dimensional Ising model: they showed that, using a peculiar transformation the two dimensional Ising model can be exactly rewritten as another two dimensional Ising model, whose temperature is a monotonically decreasing function of the temperature of the original Ising model. High temperature regions of the original Ising model are then low temperature regions in its dual, and viceversa. This transformation can actually be generalized to any abelian theory, but the result can be complicated and not immediately useful. A "successful" duality transformation bears many benefits. The theory is expressed in terms of new variables, called "disorder" variables; the original theory is mapped into a dual theory such that when the temperature of the original theory is high, the one of the dual is low. Thus, when the temperature is high, the disorder variables have small fluctuations, while the original variables have large fluctuations[4].

Hinrichsen and Rittenberg [25],[26] showed that the XY model in a transverse magnetic is self dual, i.e. after a suitable transformation, can be rewritten exactly as another XY model in a transverse field where the role of the parameters (anisotropy parameter and magnetic field) is exchanged. Following the notation in [26] we write the hamiltonian

$$\mathcal{H}_{XY} = -\frac{1}{2}\sum_j \left[\eta\sigma_j^x\sigma_{j+1}^x + \eta^{-1}\sigma_j^y\sigma_{j+1}^y + q\sigma^z + q^{-1}\sigma_{j+1}^z\right] \tag{1.71}$$

that can be rewritten, up to boundary terms, as

$$\mathcal{H}_{XY} = -\frac{1}{2}\sum_j \left[\eta\sigma_j^x\sigma_{j+1}^x + \eta^{-1}\sigma_j^y\sigma_{j+1}^y\right] - h\sum_j \sigma^z \tag{1.72}$$

where $h = \left(q + q^{-1}\right)/2$ is the magnetic field. It is possible to derive an

[4]From a field theoretic point a view, a statistical system can be regarded as a euclidean field theory (where the temperature is replaced by the coupling constant); thus duality transformations are used to map theories with large coupling constants into theories with small coupling constants

orthogonal transformation[5], depending only on the ratio q/η such that

$$\mathcal{H}_{XY}(\eta, q) = \mathcal{U}(\alpha)\,\mathcal{H}_{XY}(q,\eta)\,\mathcal{U}^{-1}(\alpha) \tag{1.73}$$

The first step is to intoduce the operators [26]

$$\tau^{x,y} = \left(\prod_{i<j} \sigma_i^z\right) \sigma_j^{x,y} \tag{1.74}$$

and define

$$\alpha = \frac{q}{\eta} \qquad\qquad \omega = \frac{\alpha^{1/2} - \alpha^{-1/2}}{\alpha^{1/2} + \alpha^{-1/2}} \tag{1.75}$$

The explicit expression for the transformation is given by the polynomial [26]

$$\mathcal{U}(\alpha) = \frac{1}{\sqrt{N}} \sum_{k=0}^{L} \omega^k G_{2k} \tag{1.76}$$

where the generators G_{2k} are defined as

$$G_n = \sum_{1 \le j_1 < j_2 < \cdots < j_n \le L} \tau_{j_1}^x \tau_{j_2}^x \cdots \tau_{j_n}^x \tag{1.77}$$

By definition $G_0 \equiv 1$ and the normalization constant N is given by

$$N = \sum_{k=0}^{L} \binom{L}{2k} \omega^{2k} = 2^{L-1} \frac{1+\alpha^L}{(1+\alpha)^L} \tag{1.78}$$

Introducing a "time ordered" product

$$T\tau_j^x \tau_k^x = \left[\begin{array}{ll} \tau_j^x \tau_k^x & j<k \\ -\tau_k^x \tau_j^x & j>k \end{array} \right. \tag{1.79}$$

the transformation can be formally expressed as a time ordered exponential [26]

$$\mathcal{U}(\alpha) = \frac{1}{\sqrt{N}} T e^{\omega G_2} \tag{1.80}$$

[5] Recall the duality transformation for the Ising model [24]

$$\mu_j^x = \prod_{k<j} \sigma_k^z \qquad\qquad \mu_j^z = \sigma_j^x \sigma_{j+1}^x$$

We finally get [26]

$$\mathcal{H}_{XY}\left(\eta,q\right)=-\frac{1}{2}\sum_{j=}^{L-1}\left[\eta\sigma_{j}^{x}\sigma_{j+1}^{x}+\eta^{-1}\sigma_{j}^{y}\sigma_{j+1}^{y}+q\sigma^{z}+q^{-1}\sigma_{j+1}^{z}\right]$$

$$=-\frac{1}{2}\sum_{j=}^{L-1}\left[q\mu_{j}^{x}\mu_{j+1}^{x}+q^{-1}\mu_{j}^{y}\mu_{j+1}^{y}+\eta\mu^{z}+\eta^{-1}\mu_{j+1}^{z}\right]=\mathcal{H}_{XY}\left(q,\eta\right) \quad (1.81)$$

where

$$\mu_{j}^{x,y}=\mathcal{U}\left(\alpha\right)\sigma_{j}^{x,y}\mathcal{U}^{-1}\left(\alpha\right) \quad (1.82)$$

are the disorder operators.

Chapter 2

Spin 1 Heisenberg spin chains

The study of quantum spin chains has a very long history, going back at least to the solution found by Bethe [27] in 1931 for the spin 1/2 case. Spin wave theory [28], [31] predicted for antiferromagnets in $d > 2$ long range order and gapless Goldstone bosons. The behavior of 1-dimensional antiferromagnets is quite different: Mermin and Wagner theorem [29], [31] states that for the quantum Heisenberg model with short range interactions, there can be no spontaneous symmetry breaking at non zero temperatures in one and two dimensions. Thus no "true" long range order is expected, but yet the Bethe ansatz solution predicts gapless excitations. In 1983 Haldane [33], [34] suggested that integer spin chains behave in a completely different way from half-integer chains: the former have a disordered ground state and a finite gap, while the latter have gapless excitations.

This chapter is organized as follows. We will first review the semiclassical limit of the quantum Heisenberg spin chain using the Holstein-Primakoff approach to spin wave theory [30], [31], showing that, while the ferromagnet has a quadratic dispersion relation and thus it is not possible to find a corresponding Lorentz invariant field theory, the antiferromagnetic chain instead has a relativistic (linear) dispersion relation and thus can have a corresponding Lorentz invariant field theory. We will then see [30], [32], [34] that the large spin, low energy, continuum limit of the antiferromagnetic quantum chain maps aproximately onto the $O(3)$ non linear σ model (NLσM) with a topological term: it is this term that makes the behavior of the integer and half-integer spin chain completely different. In the subsequent section we will briefly discuss the nonlocal string order parameter proposed by den Nijs and Rommelse in 1989 [38] to detect the hidden order of the Haldane phase, and show how the non vanishing of the string order parameter is actually a sign of the spontaneous breaking of a hidden $Z_2 \times Z_2$ symmetry [40], [41]. Finally we will work out in detail the exactly solvable spin 1 model with a spin gap and string order provided by Affleck, Kennedy, Lieb and Tasaki in 1987 [42], [43].

2.1 A semiclassical approximation: spin waves

The Heisenberg hamiltonian can be written as

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \tag{2.1}$$

where i and j are nearest neighbor sites, and

$$\left[S_i^\alpha, S_j^\beta \right] = i\epsilon^{\alpha\beta\gamma} \delta_{ij} S_j^\gamma \qquad\qquad \mathbf{S}^2 = s\,(s+1) \tag{2.2}$$

In the classical case, i.e. the spins are fixed lenght vectors, the ground state for the ferromagnet($J < 0$) is the state with all spins parallel, while for the antiferromagnet is the Néel state, i.e. antiparallel neighboring spins. Writing the Heisenberg hamiltonian in terms of the raising and lowering operators

$$S_j^\pm = S_j^x \pm i S_j^y \tag{2.3}$$

it is easy to check that the classical ground state is also the ground state for the ferromagnetic quantum chain, while the same does not hold in the antiferromagnetic case. We want to find out if, and under what conditions, the Néel state is a good aproximation to the quantum ground state. To study this problem we will perturb the Néel state in the large S limit in which the Néel state becomes the exact ground state of the quantum chain. In order to study the small fluctuations of the spins around their expectations values Holstein and Primakoff (see for instance [30]) introduced a boson operator a which represents the three spin component operators as

$$S^+ = \left(2S - a^\dagger a\right)^{1/2} a \tag{2.4}$$

$$S^- = a^\dagger \left(2S - a^\dagger a\right)^{1/2} \tag{2.5}$$

$$S^z = S - a^\dagger a \tag{2.6}$$

Expanding in $1/S$ the relations written above, plugging them into the Heisenberg hamiltonian and retaining up to quadratic terms, we get in the ferromagnetic case [30]

$$\mathcal{H}_F = JS \sum_{\langle i,j \rangle} \left[-a_i^\dagger a_i + a_j^\dagger a_j + a_i^\dagger a_j + a_j^\dagger a_i\right] \tag{2.7}$$

or in momentum space

$$\mathcal{H} = |J|Sz \sum_{\mathbf{k}} (1 - \gamma_k)\, a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \tag{2.8}$$

where

$$\gamma_{\mathbf{k}} = \frac{1}{z} \sum_{j,\langle i,j \rangle} e^{i(\mathbf{X}_j - \mathbf{X}_i)\cdot \mathbf{k}} \tag{2.9}$$

and z is the number of nearest neighbors. At small $\mathbf{k}$ we get a dispersion relation quadratic in momenta, i.e. non relativistic

$$E_{\mathbf{k}} \to JS\mathbf{k}^2 \tag{2.10}$$

This is the gapless Goldstone mode, which is a consequence of the broken symmetry of the ferromagnetic ground state. The lowest order correction to the ground state magnetization can be calculated at finite temperatures, and, while small for $d > 2$, it is divergent in $d = 1, 2$, consistently with Mermin and Wagner's theorem [29].

For the antiferromagnetic case, following Affleck [30], we consider a bipartite lattice, on one sublattice, say A, we perform the above expansion, while on sublattice B we represent the spins in terms of the boson b

$$S^z = -S + b^\dagger b \tag{2.11}$$

$$S^- = \left(2S - b^\dagger b\right)^{1/2} b \tag{2.12}$$

The state with no bosons is just the Néel state. After expanding in powers of $1/S$, keeping up to quadratic terms in the hamiltonian, going to momentum space and performing the Bogoliubov transformation

$$c_{\mathbf{k}} = u_{\mathbf{k}} a_{\mathbf{k}} - v_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} \tag{2.13}$$

$$d_{\mathbf{k}} = u_{\mathbf{k}} b_{\mathbf{k}} - v_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} \tag{2.14}$$

we get the diagonal hamiltonian[1]

$$\mathcal{H}_{AF} = JSz \sum_{k} \left(1 - \gamma_k^2\right)^{1/2} \left(c_k^{\dagger} c + d_k^{\dagger} d_k\right) \tag{2.17}$$

The excitations created by c and d are known as spin waves, they correspond to infinitesimal deviations of the spins away from the Néel state. Their dispersion relation is relativistic in the limit $k \to 0$

$$E_k \to 2JSz|k| \tag{2.18}$$

The staggered magnetization can be calculated using spin wave theory and it has been found that in $d \geq 2$ the correction is relatively small for large S; in $d = 1$ [31]

$$\Delta\langle S_z\rangle = -\frac{1}{2\pi}\int \frac{dk}{2k} = -\infty \tag{2.19}$$

i.e. the Néel order is broken by quantum fluctuations no matter how large S is, as it is expected from Mermin and Wagner's theorem.

2.2 Continuum limit of the quantum Heisenberg spin chain

We will now derive the low energy, continuum aproximation of the quantum magnet. The basic idea is to separate the long wave, low energy fluctuations and the short wave ones, "integrating out" the latter ones.

[1] The coefficients of the Bogoliubov transformation are obtained solving

$$|u_k|^2 - |v_k|^2 = 1 \tag{2.15}$$

$$\gamma_k \left(u_k^2 + v_k^2\right) + 2u_k v_k = 0 \tag{2.16}$$

The starting point to treat the large spin limit of the quantum Heisenberg chain is its canonical partition function on the coherent state basis[2] [31], [32]

$$\mathcal{Z} = \int \mathcal{D}\mathbf{\Omega} \exp\left(is\mathcal{S}_{WZ} - \int_0^\beta dt \mathcal{H}\left[\mathbf{\Omega}\right] \right) \tag{2.20}$$

where the vector operator $\mathbf{S}_j$ of the hamiltonian (2.1) has been replaced by the classical variable $\mathbf{S}_j = s\mathbf{\Omega}_j$ with the constraint $\mathbf{\Omega}_j^2 = 1$, and the Wess-Zumino term is

$$\mathcal{S}_{WZ}\left[\mathbf{\Omega}\left(\mathbf{r}\right)\right] \equiv \int_0^1 d\chi \int_0^\beta dt \mathbf{\Omega}\left(t,\chi\right) \cdot \left(\partial_t \mathbf{\Omega}\left(t,\chi\right) \times \partial_\chi \mathbf{\Omega}\left(t,\chi\right)\right) \tag{2.21}$$

2.2.1 Quantum ferromagnets

We first consider the ferromagnetic case on a hyper cubic lattice. The real time[3] action can be written, up to an additive constant, as [32]

$$\mathcal{S}_F[\mathbf{\Omega}] = s \sum_{\mathbf{r}} \mathcal{S}_{WZ}\left[\mathbf{\Omega}\left(\mathbf{r}\right)\right] + \frac{Js^2}{2} \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} \int_0^T d\tau \left[\mathbf{\Omega}\left(\mathbf{r},\tau\right) - \mathbf{\Omega}\left(\mathbf{r}',\tau\right)\right]^2 \tag{2.22}$$

In the long wavelenght limit $\mathbf{\Omega}\left(\mathbf{r},\tau\right)$ is a smooth function of the spatial variables, thus in this limit the action reads

$$\mathcal{S}_F[\mathbf{\Omega}] = \frac{s}{a} \int d^d x \mathcal{S}_{WZ}\left[\mathbf{\Omega}\right] + \frac{Js^2}{2a^{d-2}} \int d^d x \int_0^T d\tau \left[\nabla_i \cdot \mathbf{\Omega}\left(x,\tau\right)\right]^2 \tag{2.23}$$

Thus the effective continuum action for the quantum antiferromagnet does not have the non linear σ model form, as we should have expected, since the large s limit of the ferromagnet has a quadratic dispersion relation, and thus it cannot be put in correspondence with a Lorentz invariant field theory. It is also consistent with the fact that NLσM leads to Goldstone bosons with a linear dispersion relation, while ferromagnetic magnons have a quadratic dispersion relation.

2.2.2 Quantum antiferromagnets

We will consider a spin chain with antiferromagnetic coupling constant $J > 0$ with an even number of sites on a bipartite lattice. The real time

[2] For a brief introduction to spin coherent states see for example [31]

[3] We make a Wick rotation $t = i\tau$

action is [32]

$$\mathcal{S}_{AF} = s\sum_{j=1}^{N}\mathcal{S}_{WZ}[\mathbf{\Omega}_j] - \int_0^t d\tau \sum_{j=1}^{N} Js^2\mathbf{\Omega}_j(\tau)\cdot\mathbf{\Omega}_{j+1}(\tau) \tag{2.24}$$

where we assumed periodic boundary conditions. Since we expect to be close to the Néel state we stagger the configuration $\mathbf{\Omega}_j \rightarrow (-1)^j\mathbf{\Omega}_j$. The effect of this transformation on a bipartite lattice is to change the sign of the exchange term to a ferromagnetic one, while Wess-Zumino terms get staggered. The effective action thus becomes, up to a constant

$$\mathcal{S}_{AF} = s\sum_{j=1}^{N}(-1)^j\mathcal{S}_{WZ}[\mathbf{\Omega}_j] - \int_0^t d\tau \sum_{j=1}^{N} Js^2\left(\mathbf{\Omega}_j(\tau) - \mathbf{\Omega}_{j+1}(\tau)\right)^2 \tag{2.25}$$

We now define [32]

$$\mathbf{\Omega} = \mathbf{n}_j + (-1)^j a\mathbf{l}_j \tag{2.26}$$

where the two fields satisfy the constraints

$$\mathbf{n}^2 = 1 \qquad\qquad \mathbf{n}\cdot\mathbf{l} = 0 \tag{2.27}$$

The Wess-Zumino term becomes then in the continuum limit

$$\lim_{a\to 0} s\sum_{j=1}^{N}(-1)^j\mathcal{S}_{WZ}[\mathbf{\Omega}_j] \simeq \frac{s}{2}\int dx d\tau\, \mathbf{n}\cdot(\partial_\tau\mathbf{n}\times\partial_x\mathbf{n})$$

$$+s\int dx d\tau\, \mathbf{l}\cdot(\mathbf{n}\times\partial_\tau\mathbf{n}) \tag{2.28}$$

Similarly the continuum limit of the energy term becomes

$$\lim_{a\to 0}\int_0^t d\tau\sum_{j=1}^{N} Js^2\left(\mathbf{\Omega}_j(\tau) - \mathbf{\Omega}_{j+1}(\tau)\right)^2$$

$$\simeq \frac{aJs^2}{2}\int dx d\tau\,\left(\partial_x\mathbf{n} + \mathbf{l}\right)^2 \tag{2.29}$$

Collecting terms, we find the lagrangian density [32]

$$\mathcal{L}[\mathbf{n},\mathbf{l}] = -2ajs^2\mathbf{l}^2 + s\mathbf{l}\cdot(\mathbf{n}\times\partial_\tau\mathbf{n}) - \frac{aJs^2}{2}\left(\partial_x\mathbf{n}\right)^2 + \frac{s}{2}\mathbf{n}\cdot(\partial_\tau\mathbf{n}\times\partial_x\mathbf{n}) \tag{2.30}$$

Integrating out the fluctuations over the uniform component of the spin density $\mathbf{l}$, we get the lagrangian density of the NLσM [32], [34]

$$\mathcal{L}[\mathbf{n}] = \frac{1}{2g}\left(\frac{1}{v}\left(\partial_\tau \mathbf{n}\right)^2 - v\left(\partial_x \mathbf{n}\right)^2\right) + \frac{\theta}{8\pi}\epsilon^{\mu\nu}\mathbf{n}\cdot\left(\partial_\mu \mathbf{n}\times\partial_{nu}\mathbf{n}\right) \tag{2.31}$$

where g and v are the coupling and spin wave velocity

$$g = \frac{2}{s} \qquad\qquad v = 2aJs \tag{2.32}$$

and the θ term is

$$\theta = 2\pi s \tag{2.33}$$

Let's parametrize the field with the coordinates for the sphere

$$\mathbf{n} = (\sin\alpha\cos\beta, \sin\alpha\sin\beta, \cos\alpha) \tag{2.34}$$

The Lagrangian becomes (setting here $v = 1$) [30]

$$\mathcal{L} = \frac{1}{2g}\left[\left(\partial_\mu\alpha\right)^2 + \sin^2\alpha\left(\partial_\mu\beta\right)^2\right] + \frac{\theta}{8\pi}\sin\alpha\epsilon^{\mu\nu}\partial_\mu\alpha\partial_\nu\beta \tag{2.35}$$

We see that the θ term is a total derivative and then it has no effect on the classical equation of motion and in a perturbative treatment. It leads to a change in the hamiltonian. The effect of the topological is to redefine the conjugate momenta by a canonical transformation

$$\Pi_a \rightarrow \exp i\frac{\theta}{4\pi}\int dx\beta'\cos\alpha\Pi_a \exp -i\frac{\theta}{4\pi}\int dx\beta'\cos\alpha \tag{2.36}$$

Thus the θ dependance of the hamiltonian can be removed making the above transformation. However it is expected that the Hilbert space breaks into sectors labeled by θ. Performing the canonical transformation on the states corresponds to a map between the different sectors, in particular between the different ground states called θ vacua.

2.2.3 The topological θ term

Let's consider the Euclidean ($\tau = it$) lagrangian

$$\mathcal{L}[\mathbf{n}] = \frac{1}{2g}\left(\frac{1}{v}\left(\partial_t \mathbf{n}\right)^2 + v\left(\partial_x \mathbf{n}\right)^2\right) + i\frac{\theta}{8\pi}\epsilon^{\mu\nu}\mathbf{n}\cdot\left(\partial_\mu \mathbf{n}\times\partial_\nu\mathbf{n}\right) \tag{2.37}$$

The topological term

$$\mathcal{Q} = \frac{1}{8\pi} \int d^2x \epsilon^{\mu\nu} \mathbf{n} \cdot (\partial_\mu \mathbf{n} \times \partial_{nu} \mathbf{n}) \tag{2.38}$$

is the Pontryagin index [45] of the Euclidean space spin configuration $\{\mathbf{n}(x)\}$. We require the Euclidean action to be finite, i.e. $\mathbf{n}(x)$ becomes a constant vector $\mathbf{n}_0$ at infinity. Topologically the Euclidean space time is a sphere S^2 since the fields are identified with a constant at the point of infinity; the order parameter manifold is also isomorphic to S^2 since the constraint $\mathbf{n} = 1$ must hold everywhere. Thus, a field configuration with a finite euclidean action is a smooth mapping from S^2 to S^2.

Field configurations can then be classified according to their winding number. In other words, the field configurations $\mathbf{n}$ are mappings from S^2 into S^2 with homotopy classes classified by an integer, the Pontryagin index $\mathcal{Q}$, i.e. the second homotopy group [45]

$$\pi_2(S^2) = \mathbb{Z} \tag{2.39}$$

The partition function of the Heisenberg model in the large S limit $\mathcal{Z} = \exp(-i\mathcal{S}_{AF})$ has a contribution due to the NLσM at $\theta = 0$ and an additional topological term $\exp i2\pi s\mathcal{Q} = (-1)^{2s\mathcal{Q}}$. Then, if the spin is integer the topological term is 1 and the Heisenberg chain is described at low energies by the pure NLσM. For half-integral spin, each topological class contributes with a sign which is positive or negative if the Pontryagin index is even or odd. This property is the very motivation of the different behavior of the two kinds of chains.

2.2.4 Renormalization group

We will now consider the role of quantum fluctuations. Assuming fluctuations to be local and reasonably small, it is possible to treat the path integral semiclassically; this can be actually done only if the coupling constant $g = 2/s$ is small, i.e. in the large s limit. A very important property of the classical action of the NLσM is that it is scale invariant; from renormalization group theory it is known [46] that, if the action is scale invariant, then the point $g = 0$ is a fixed point for the renormalization group (RG).

From RG it can be obtained the β function [32]

$$\beta(u) = -\epsilon u + \frac{u^2}{2\pi} + O(u^3) \tag{2.40}$$

where u is the dimensionless coupling $u = ga^{2-d}$, $\epsilon = d - 2$ and a is the lattice spacing. The β function actually measures the change of the coupling constant u as the cutoff a is increased and the fast degrees of freedom of the system are progressively integrated out.

In particular, in $1 + 1$ dimensions the β function is positive [47]

$$\beta(u) = \frac{u^2}{2\pi} \tag{2.41}$$

This means that as the cutoff a is increased the fluctuations increase the effective value of the coupling constant. Thus even if the bare coupling u_0 is small, it increases as we consider the effective theory at low energies. It is known from classical statistical mechanics that the NLσM at strong coupling is disordered and has finite correlation length. That is, in the "spin picture" as the spin gets small, the semiclassical behavior is destroyed, and we find a state with no spontaneous symmetry breaking and short range correlations.

Let's keep the lattice constant fixed and vary an energy scale such as the temperature T instead. At finite temperature T the system can be viewed as a NLσM on a strip of length L (the length of the chain) and width $1/T$ with periodic boundary conditions in imaginary time. We start our RG process with some fixed cutoff a_0, bare coupling u_0 and spin velocity v. Integrating out degrees of freedom, the effective coupling u and the spatial cutoff a increase. When the spatial cutoff $a \simeq v/T$, i.e. it is as large as the width of the strip, the quantum fluctuations are negligible and we have a NLσM at some finite temperature T. It is now interesting to see how the coupling constant u differs from u_0 when the cutoff is changed from a_0 to $a_1 \simeq v/T$. Solving the differential equation

$$\beta(u) = a_0 \frac{du}{da_0} = \frac{u^2}{2\pi} \tag{2.42}$$

and choosing $a_1 \simeq v/T$, the temperature dependance of the effective coupling is given by [47]

$$u(T) = \frac{u_0}{1 + \frac{u_0}{2\pi} \ln\left(\frac{aT}{v}\right)} \tag{2.43}$$

This result is known as asymptotic freedom, i.e. the coupling constant is small at high temperatures or small distances.

Using RG we can finally calculate the dependance of the correlation length ξ on the coupling constant. It is found that [31], [32]

$$\xi(u_0) \simeq \xi(u')e^{\pi s} \tag{2.44}$$

whit u' a large value of the coupling constant with the same a as u_0. The limiting value $\xi(u')$ as $u' \to \infty$ depends on wheter s is integer or half integer

- For the integer spin case there is no topological term. The sigma model is always disordered at strong coupling, and then we expect $\xi(u') \simeq a$. Thus we have a finite correlation length

$$\xi(u_0) \simeq ae^{\pi s} \tag{2.45}$$

  there is no long range order, the spectrum has a gap $\Delta = v/\xi(u_0)$ and ground state is unique

- For the half integer case the topological term remains unchanged at the value $\theta = 2\pi s$. The coupling constant is related to the spin s by $u = 2a^{2-d}/s$, thus strong coupling is equivalent to small spin. We have then that the behavior for all half integer chains is qualitatively identical to the spin 1/2 case. This case is gapless, thus $\xi(\infty)$ is infinite. All half integral chains are then gapless with infinite correlation length.

2.3 String order parameter

Haldane's conjecture that antiferromagnetic integer spin chain at their isotropic Heisenberg point have a disordered ground state, with massive excitations is now commonly accepted. The existence of this phase which presents a hidden antiferromagnetic order and is different from the Néel phase led people to propose "new" order parameters able to distinguish the Haldane phase. In 1987 den Njis and Rommelse [39], studying the roughening of crystal surfaces in the Restricted Solid on Solid(RSOS) model, discovered a new phase which they called the disordered flat phase(DOF); in this phase the surface is on average flat, altough it shows disordered arrays of

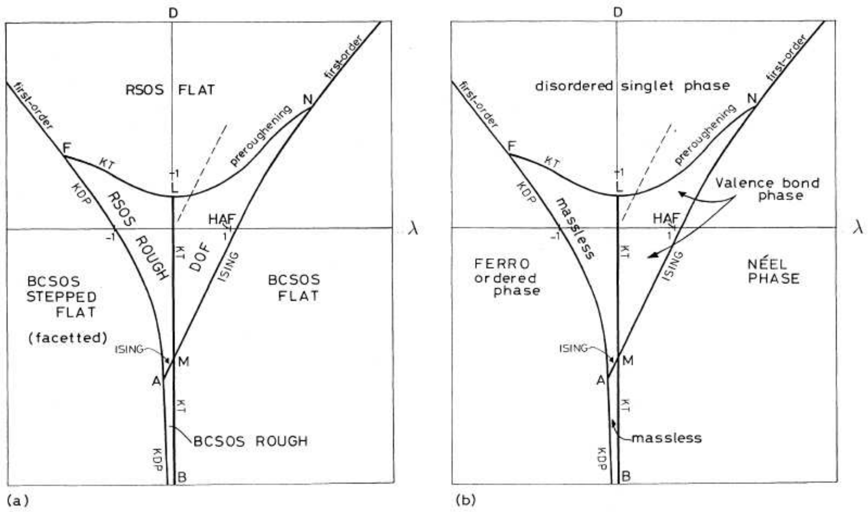

Figure 2.1: Phase diagram [38] of the spin 1 λ - D model using (a) the RSOS language, and (b) the spin 1 language

steps, having long range up down order. To distinguish the various phases of the phase diagram of the RSOS they introduced correlation functions and order parameters [38]. They then proved that the transfer matrix of the RSOS model is equivalent to that of a very general spin 1 hamiltonian with nearest neighbor interactions, that under particular assumptions is just the λ-D model. Under these assumptions they then made explicit the correspondence between phases in the RSOS and the spin 1 λ-D model (2.52), finding out in particular that the DOF phase corresponds to the Haldane phase.

They interpreted the spin 1 chain as a diluted spin 1/2. The site is empty, the $S^z = 0$ state, or occupied by a spin 1/2 particle, with the states $S^z = \pm 1$ representing the spin of the particle. These particles behave then like a solid, a liquid or a gas in the various regions of the phase diagram; the Néel phase has perfect antiferromagnetic order with no empty sites, and can be depicted as a solid. The Haldane phase can be regarded as a liquid in the sense that there is no positional order but there is long range antiferromagnetic order. Finally the large D phase is interpreted as a gas since there is no order left.

They then "translated" correlators and order parameter in the spin language. They found in particular that the step-step correlation function, which does not vanish in DOF, can be written as the so called string order parameter [38]

$$\mathcal{O}^z_{i,j} = \langle 0|S^z_i e^{i\pi \sum_{k<j} S^z_k} S^z_j|0\rangle \tag{2.46}$$

This non local correlator is not vanishing in the Haldane as well as the in the Néel phase. In order to get an idea of what this order parameter measures, let's remind [42] that the ground state of the Haldane phase can be written as a Valence Bond Solid (VBS)[4]. We then consider an allowed VBS ground state configuration

$$|VBS\rangle = |\cdots + 000 - 0 + - + 0 \cdots 0 - + \cdots\rangle \tag{2.47}$$

This configuration does not have long range order: if we fix the spin at a given site we are not able to say what will be the spin at another site; however if we keep track of the number of non zero spins from the reference site we can predict what the spin at a distant site will do. This is exactly what the exponential in the string order parameter does, it gives a ± 1 wheter there is an even (odd) number of non zero sites between the two reference sites.

2.3.1 Hidden symmetry breaking and the string order parameter

Kennedy and Tasaki [40], [41] showed that the hidden order measured by the string order parameter is due to the breaking of a hidden $Z_2 \times Z_2$ symmetry.

We consider a finite chain with an even number sites and impose boundary conditions. Let $\sigma = \{\sigma_i\}$ be a choice of $\sigma_i = -1, 0, +1$ at each site i, and Φ_σ denotes the eigenstate with $S^z_i \Phi_\sigma = \sigma_i \Phi_\sigma$. Denote $N(\sigma)$ to be the number of odd sites at which there is a 0, and let $\bar{\sigma}$ be the configuration

$$\bar{\sigma}_i = e^{i\pi \sum_{k<j} \sigma_j} \tag{2.48}$$

[4]See Sec.2.4 for more details on VBS

We define the unitary $\mathcal{U}$ by [40], [41]

$$\mathcal{U}\Phi_\sigma = (-1)^{N(\sigma)}\Phi_{\bar{\sigma}} \tag{2.49}$$

If $\sigma_i = 0$ then $\bar{\sigma}$. If $\sigma_i \neq 0$, then $\bar{\sigma}_i = \sigma_i$ if the number on nonzero σ_l to the left of i is even and $\bar{\sigma}_i = -\sigma_i$ if this number is odd. Beginning from the left of the chain we move to the right looking for nonzero spins: the first non zero spin is left unchanged, the second is flipped, the third is unchanged and so on. As an example of the action of the unitary

$$|\cdots 0 + -0000 + +0 - 0 + 00 + - \cdots\rangle \rightarrow |\cdots 0 + +0000 + -0 - 0 - 00 + + \cdots \rangle \tag{2.50}$$

It is immediate from the definition that $\mathcal{U}$ is unitary. It can be shown that the transformation can also be expressed as

$$\mathcal{U} = \prod_{j<k} e^{i\pi S_j^z S_k^x} \tag{2.51}$$

The unitary is non local, in the sense that it cannot be written as a product of unitary operators acting at each single site. Let's see how the λ-D hamiltonian

$$\mathcal{H} = \sum_{i=1} L \left[\mathbf{S}_i \cdot \mathbf{S}_{i+1} + (\lambda - 1)\, S_i^z S_{i+1}^z + D\,(S_i^z)^2\right] \tag{2.52}$$

transforms under the action of the unitary. The term $D\,(S_i^z)^2$ is left unchanged since this term does not distiguish between $\sigma_i = 1$ and $\sigma_i = -1$. For $S_i^z S_{i+1}^z \Phi_\sigma$ to be non vanishing, both σ_i and σ_{i+1} must be non zero. If so, exactly one of these two sites must be flipped. Thus this term acquires a $-$ sign. To see how the off diagonal part changes, we must take into account that $S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+$ conserves the number of non zero spins of each configuration σ or changes it by two. Since the unitary only involves the parity of the number of non zero spins on the left of a site i, the above hamiltonian elements do not affect the unitary at the k-th site for $k > i + 1$. Thus the matrix elements $\mathcal{U}\left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+\right)\mathcal{U}^{-1}$ are still local. It can be shown that [40], [41]

$$\tilde{\mathcal{H}} = \sum_{i=1}^{L} \left[h_i + (1 - \lambda)\, S_i^z S_{i+1}^z + D\,(S_i^z)^2\right] \tag{2.53}$$

where

$$h_i = -S_i^x S_{i+1}^x + S_i^y e^{i\pi\left(S_i^x + S_{i+1}^x\right)} S_{i+1}^y - S_i^z S_{i+1}^z \tag{2.54}$$

The $SO(2)$ symmetry of the original hamiltonian is destroyed by the unitary. We find that $\tilde{\mathcal{H}}$ is only invariant under rotations of π about each of the three coordinate axes. These three rotations generate the discrete group $Z_2 \times Z_2$. The transformed hamiltonian has the the same symmetries of the original hamiltonian $\mathcal{H}$ since they are related by the unitary, but in general, these symmetries for $\tilde{\mathcal{H}}$ will be non local. The only local symmetry of the transformed hamiltonian is the discrete $Z_2 \times Z_2$ symmetry. This can be thought of as generated by the rotations of π around the axes x and z. Kennedy and Tasaki [40], [41] also showed how the Néel order parameter, the ferromagnetic order and the string order parameter

$$\mathcal{O}_{Neel}^{\alpha}\left(\mathcal{H}\right) = \lim_{|i-j|\to\infty} (-1)^{|i-j|} \langle S_i^{\alpha} S_{i+1}^{\alpha} \rangle \tag{2.55}$$

$$\mathcal{O}_{ferro}^{\alpha}\left(\mathcal{H}\right) = \lim_{|i-j|\to\infty} \langle S_i^{\alpha} S_{i+1}^{\alpha} \rangle \tag{2.56}$$

$$\mathcal{O}_{string}^{\alpha}\left(\mathcal{H}\right) = \lim_{|i-j|\to\infty} -\langle S_i^{\alpha} e^{i\pi \sum_{k=i+1}^{j-1}} S_{i+1}^{\alpha} \rangle \tag{2.57}$$

transform under the unitary transformation $\mathcal{U}$

$$\mathcal{O}_{string}^{\alpha}\left(\mathcal{H}\right) = \mathcal{O}_{ferro}^{\alpha}\left(\tilde{\mathcal{H}}\right) \qquad \text{for} \qquad \alpha = x, z \tag{2.58}$$

Possible spontaneous breaking of the discrete symmetry $Z_2 \times Z_2$ can be measured by the order parameters $\mathcal{O}_{ferro}^{x}\left(\tilde{\mathcal{H}}\right)$ and $\mathcal{O}_{ferro}^{z}\left(\tilde{\mathcal{H}}\right)$

Let's consider the various phases of the model. When $|\lambda - D| \gg 1$ we know that the hamiltonian has two infinte volume ground states with long range Neel order. We have $\mathcal{O}_{Neel}^{z}\left(\mathcal{H}\right) > 0$ and $\mathcal{O}_{string}^{z}\left(\mathcal{H}\right) > 0$, while $\mathcal{O}_{Neel}^{\alpha}\left(\mathcal{H}\right) = \mathcal{O}_{Neel}^{\alpha}\left(\mathcal{H}\right) = 0$ for $\alpha = x, y$. This is consistent with the fact that in this limit the transformed hamiltonian describes a ferromagnetic Ising chain with a small perturbation. This hamiltonian has two infinite volume ground states where the $Z_2 \times Z_2$ symmetry is partially broken: the Z_2 symmetry corresponding to rotations about the x axis is spontaneously broken, while the other Z_2 is left unbroken.

In the large D phase the infinite volume ground state of $\mathcal{H}$ is unique, has exponentially decaying correlation functions and has a finite gap. All order parameters are vanishing. The ground state of $\tilde{\mathcal{H}}$ has similar properties and breaks no symmetry.

Let's turn finally to the Haldane phase. The ground state is unique, has exponentially decaying correlation functions and has a finite gap, but, as argued by den Njis and Rommelse [38], it is believed to have a hidden antiferromagnetic order: $\mathcal{O}^{\alpha}_{Neel}(\mathcal{H}) = 0$ for $\alpha = x, y, z$ but $\mathcal{O}^{\alpha}_{string}(\mathcal{H}) > 0$ for $\alpha = x, y, z$. For the transformed hamiltonian $\tilde{\mathcal{H}}$ we have $\mathcal{O}^{\alpha}_{ferro}\left(\tilde{\mathcal{H}}\right) = 0$ for $\alpha = x, z$ and the full symmetry $Z_2 \times Z_2$ is spontaneously broken.

2.4 An exactly solvable example: the AKLT model

In this section we will show the first example of an exactly solvable one dimensional spin one hamiltonian with a unique ground state with no broken symmetries[5,6]. The key idea to this model is the notion of valence bond. Given two spin 1/2 a valence bond is formed by putting them into the singlet state $\uparrow\downarrow - \downarrow\uparrow$. Consider now the spin 1 chain: each spin 1 at site i can be regarded as the symmetric part of two spin 1/2. The state will be constructed with a valence bond between each pair of adjacent sites i and $i+1$ by forming a singlet out of one spin 1/2 at site i and one spin 1/2 at site $i+1$. The next step is to symmetrize the two spin 1/2 at each site. The resulting state will be called Valence Bond Solid (VBS) [42].

Let's now show in detail the construction of the model. Denote the sites of the lattice by i and the spin $s = 1$ operators at site i by $\mathbf{S}_i$. The restriction of a state to two neighboring sites can have total spin 0, 1 or 2. The orthogonal projection onto states with spin 2 can be written in terms of spin operators as [42]

$$\mathcal{P}_2\left(\mathbf{S}_i + \mathbf{S}_{i+1}\right) = \frac{1}{2}\left[\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{3}\left(\mathbf{S}_i \cdot \mathbf{S}_{i+1}\right)^2 + \frac{2}{3}\right] \tag{2.59}$$

[5] The procedure used to construct this model can actually be generalized to dimensions bigger than one and generic spin s whenever $2s$ equals the coordination number of the lattice [42]

[6] We will see that a hidden $Z_2 \times Z_2$ symmetry is actually broken

The hamiltonian will be the sum over i of these projections

$$\mathcal{H} = \sum_i \mathcal{H}_i = \sum_i \mathcal{P}_2 \left(\mathbf{S}_i + \mathbf{S}_{i+1}\right) \tag{2.60}$$

This hamiltonian is positive semi-definite, so we can find a ground state Ω, i.e. $\mathcal{P}_2 \left(\mathbf{S}_i + \mathbf{S}_{i+1}\right) \Omega = 0$ for all i.

Following [43] we introduce a special basis for the state space. Let's consider first the state space for a single spin 1/2 and denote with ψ_1 and ψ_2 the eigenstates of S^z with eigenvalues $+1/2$ and $-1/2$. The state space for spin 1 may be constructed by taking the symmetric part of the tensor product of two spin 1/2 spaces. Thus an orthogonal basis can be written as

$$\psi_{\alpha\beta} = \frac{1}{\sqrt{2}} \left[\psi_\alpha \otimes \psi_\beta + \psi_\beta \otimes \psi_\alpha\right] \qquad \alpha, \beta = 1, 2 \tag{2.61}$$

with $\psi_{\alpha\beta} = \psi_{\beta\alpha}$. These states are not all normalized to 1, in fact we have

$$(\psi_{\alpha\beta}, \psi_{\gamma\delta}) = \psi^{\dagger\alpha\beta} \cdot \psi_{\gamma\delta} = \delta^\alpha_\gamma \delta^\beta_\delta + \delta^\alpha_\delta \delta^\beta_\gamma \tag{2.62}$$

where we have raised indices in order to make the $SU(2)$ invariance of the theory more explicit.

There are four spin 1/2 associated with each bond of the chain. If two of these spin 1/2 are in a singlet state, then the four spins can have at most spin 0 or 1. A singlet pair is formed by contracting with the antisymmetric tensor $\epsilon^{\alpha\beta}$, i.e. $\psi_\alpha \otimes \psi_\beta \epsilon^{\alpha\beta}$ (the sum over repeated upper and lower indices is assumed). Given two spin 1 we can write $\Omega_{\alpha\beta} = \psi_{\alpha\gamma} \otimes \psi_{\delta\beta} \epsilon^{\gamma\delta}$; since in this state two spins 1/2 will always be in a singlet state, we will have that $\Omega_{\alpha\beta}$ will always be a mixture of states with total spin 0 and 1 [43]. We have then found that $\Omega_{\alpha\beta}$ is a ground state for the projector onto spin 2.

We can now write down the ground state of the hamiltonian (2.60) of a finite chain with an odd number of sites L (the definition is essentialy the same if L is even) [43]

$$\Omega_{\alpha\beta} = \psi_{\alpha\beta_1} \otimes \psi_{\alpha_2\beta_2} \otimes \cdots \otimes \psi_{\alpha_{L-1}\beta_{L-1}} \otimes \psi_{\alpha_L\beta} \epsilon^{\beta_1\alpha_2} \epsilon^{\beta_2\alpha_3} \cdots \epsilon^{\beta_{L-1}\alpha_L} \tag{2.63}$$

For any two neighboring sites i and $i+1$ there is a spin 1/2 at site i and a spin 1/2 at site $i+1$ which are contracted by an antisymmetric tensor to form a singlet. Then, when $\Omega_{\alpha\beta}$ is restricted to two adjacent sites it can

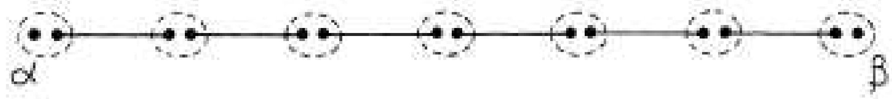

Figure 2.2: The VBS state [43]. Each dot, line and dotted circle represents a spin 1/2, a singlet pair and two symmetrized spin 1/2

have only spin 0 and 1. Thus it is a ground state for $\mathcal{H}_i$ for all i and so is a ground state of the hamiltonian (2.60).

We can give a pictorial representation of the VBS ground state (see Fig. 2.2). Each site is represented as two dots, with each dot representing a spin 1/2. The bold line connecting two neighboring dots represents a singlet state. After forming these singlets we symmetrize the two spin at each site. This is done by the dotted circles.

Despite being written in a very compact form, VBS ground states are not at all trivial; for instance, they cannot be written as tensor product states of single site states. Let's express the VBS state in terms of eigenstates of S^z that is in terms of $\{|+\rangle = \psi_{11}/\sqrt{2}, |0\rangle = \psi_{12} = \psi_{21}, |-\rangle = \psi_{22}/\sqrt{2}\}$. The basis vectors for the chain are labelled by strings of $+$, 0 and $-$. These strings will be denoted by A, the corresponding state by ψ_A and its coefficient in the ground state $\Omega_{\alpha\beta}$ will be $\Omega_{\alpha\beta}(A)$. This coefficient is zero unless the string is in a very special form depending on α and β. In particular [43]

- $\alpha = 1$, $\beta = 2$. A must contain the same number of $+$ and $-$; the first non zero character in A must be a $+$, and the non zero characters must alternate between $-$ and $+$.

- $\alpha = 2$, $\beta = 1$. Same as above with $+$ and $-$ reversed.

- $\alpha = 1$, $\beta = 1$. A must contain one more $+$ than $-$; the first non zero character in A must be a $+$, and the non zero characters must alternate between $-$ and $+$.

- $\alpha = 2$, $\beta = 2$. Same as above with $+$ and $-$ reversed.

These four cases are disjoint except this case: the string containing all 0 belongs to the classes with $\alpha = 1$, $\beta = 2$ and $\alpha = 2$, $\beta = 1$. It can be shown however that in the infinite volume limit [43] these four ground states converge to a single infinite volume ground state.

Interestingly enough, Arovas, Auerbach and Haldane [44] have shown, using the Schwinger boson representation of the spin algebra[7][31], that the VBS ground state (2.63) can be expressed for abitrary spin S and lattice $\mathcal{L}$ as

$$\Omega(u,v) = \prod_{\langle i,j \rangle} (u_i v_j - v_i u_j)^M \tag{2.64}$$

with $S = Mz/2$, z being the coordination number of the lattice, showing in this way a striking analogy between this wave function and the Laughlin wave function

$$\Psi = \prod_{j<k} (z_j - z_k)^m \exp\left\{ -\frac{1}{4} \sum_l |z_l|^2 \right\} \tag{2.65}$$

which describes the fractional quantum Hall condensate at filling fraction $\nu = 1/m$ (m odd).

Having found the explicit expression of the ground state (2.63) it is possible to calculate the spin correlation functions [43]

$$\langle S_0^a S_R^b \rangle = (-1)^R \delta^{ab} \frac{4}{3} 3^{-R} \tag{2.66}$$

thus the correlation functions decay exponentially with correlation length $\xi = 1/\ln 3$. The string order parameter is found to be [41]

$$\lim_{R\to\infty} \langle S_0^a e^{i\pi \sum_{k=1}^{R-1} S_k^a} S_R^a \rangle = \frac{4}{9} \qquad a = x, z \tag{2.67}$$

Furthermore it is possible to show [43] that the ground states constructed above are the only ground states, and that in the infinite volume limit there is a gap between the ground state and the first excited state.

Finally, we notice that the hamiltonian (2.60) is a special case of the more general

$$\mathcal{H} = \sum_i \left[\mathbf{S}_i \mathbf{S}_{i+1} - \beta \left(\mathbf{S}_i \mathbf{S}_{i+1} \right)^2 \right] \tag{2.68}$$

[7]Taking $a^\dagger \to u = \cos(\theta/2)e^{i\phi}$ and $b^\dagger \to v = \sin(\theta/2)e^{i\phi}$, $a \to \partial_u$ and $b \to \partial_v$, where a and b are the Schwinger bosons as defined in [31]

This model has been solved for $\beta = 1$ with the Bethe ansatz method [36], [37]. It has a unique ground state with no gap and power law decaying correlation functions. It has been argued [42] that $\beta = 1$ is a critical point separeting the VBS phase[8],and dimerized phases (respectively for $\beta < 1$ and $\beta > 1$).

[8]The phase with a unique ground state, exponential decay and a gap

Chapter 3

Effective mapping

3.1 Introduction

The Haldane phase [41], found in many low-dimensional spin systems, has attracted a great amount of attention in the last two decades both from the theoretical and from the experimental points of view. Its genuine quantum nature is signalled by two characteristic features. First, the excitation spectrum above the ground state (GS) displays a finite energy gap and, second, one can identify suitable long-ranged string correlation functions that measure a hidden topological order of the phase. The most intuitive idea to understand the physical features of the Haldane phase is probably the *spin liquid* picture [48]: In a spin-1 chain with Heisenberg interactions and quantization axis directed along z, let us assign the presence of an effective spin-1/2 particle with spin pointing up (down) if at the i-th lattice site $S_i^z = +1$ (-1) and no particles if $S_i^z = 0$. The Haldane phase is then interpreted as a liquid in which these effective particles carry no positional order along the chain but still retain antiferromagnetic (AFM) order in their effective spins. The positional disorder is associated with the absence of long-range order in the usual spin-1 correlation functions

$$\mathcal{C}_\alpha(R) \equiv (-1)^R \langle S_i^\alpha S_{i+R}^\alpha \rangle \ , \quad \alpha = x, y, z$$

whereas the spin-1/2 magnetic order that we would get if all the sites with $S_i^z = 0$ were taken off from the chain is measured by the asymptotic value of the string correlators [38]:

$$\mathcal{O}_\alpha(R) \equiv \langle S_i^\alpha \mathrm{e}^{\mathrm{i}\pi \sum_{j=i+1}^{i+R-1} S_j^\alpha} S_{i+R}^\alpha \rangle \ , \quad \alpha = x, y, z \tag{3.1}$$

for $R \to \infty$. Interestingly enough, the Haldane gap has been interpreted as the excitation energy associated with a "spinon" (or kink) with respect to the hidden order [49]. The nonvanishing values of the string-order parameters (SOP)

$$\mathcal{O}_\alpha \equiv \lim_{R\to\infty} \mathcal{O}_\alpha(R)$$

can be understood as a spontaneous breaking of hidden (nonlocal) Z_2 symmetries of the $\lambda - D$ Hamiltonian, as discussed thoroughly by Kennedy and Tasaki [41]. From a numerical inspection of the string correlation functions (3.1) computed on the first excited state with $S^z_{\mathrm{tot}} = 1$, rather than on the GS, Elstner and Mikeska [49] argued that this excited wave function is characterized by a transition region with vanishing string correlations that connects two asymptotic limits with symmetry breaking and different values of the hidden order. In a field-theoretic approach to spin-1/2 Heisenberg chain [50] such a kink is described as an effective particle - a soliton - moving with relativistic dispersion relation. When the system is moved away from criticality, due to the action of a relevant field, the soliton acquires a nonvanishing mass or an energy gap, in the condensed matter language. In ref. [51] it has been proposed a picture of the states that form the Haldane triplet at the isotropic point in terms of massive solitons and their bound states arising in the sine-Gordon formulation, valid in the neighbourhood of the critical line that marks the limit of the Haldane phase towards the large-D one (see below). The first solid numerical evidence of a nonzero Haldane gap has been provided by White and Huse [52] using the by now celebrated density-matrix renormalization group (DMRG) method.

Actually, the Haldane phase is not restriced to spin-1 systems and can be found, for example, in spin-S Heisenberg chains for every integer value of S. According to ref. [53] the gap vanishes as the classical limit $S \to \infty$ is approached as $\Delta \propto S^{-1} \exp(-\pi S)$ while the behaviour of the string order is more subtle: in order to have a nonzero value one has to generalize the string correlation function of equation (3.1) using not π in the exponential but S-dependent optimal angles $\theta_n = (2n+1)\pi/S$ with $n = 0, 1, \ldots, S-1$. Again, when $S \to \infty$ the resulting values of $\mathcal{O}_\alpha(\theta_n)$ tend to zero.

It is interesting to examine also how the features of the Haldane phase are destroyed by varying the parameters of the Hamiltonian out of the isotropic spin-S Heisenberg model (S integer). In this chapter we shall stick from now on to the case $S = 1$ and consider two types of anisotropies along z: Ising-like interactions (parametrized by λ) and single-ion terms (parametrized by D)

$$\mathcal{H} = \sum_i \vec{S}_i \cdot \vec{S}_{i+1} + (\lambda - 1) S_i^z S_{i+1}^z + D (S_i^z)^2. \tag{3.2}$$

The phase diagram of this model has been investigated in various papers with different approaches [41, 38, 54]. In order to fix the ideas we will refer to a recent determination [51], reported (in a simplified form) in figure 3.1. Fixing a nonnegative value for λ and varying D we encounter three gapped phases: the Large-D one in which $\mathcal{O}_\alpha = 0$ $\forall \alpha$ indicating the absence of magnetic order in the effective spin-1/2 particles. Their positional degrees of freedom are also disordered. In the Haldane phase the spatial disorder persists but magnetic order emerges. As a consequence both longitudinal and transverse string order parameters (SOP) become nonzero: $\mathcal{O}_\alpha \neq 0$. As pointed out in ref. [55] on the basis of an exact solution for an integrable variant of (3.2) with $\lambda = 0$ and in-plane anisotropy, the excitation gaps in the Large-D and in the Haldane phases have a rather different nature. Despite the fact that they are both found within the sector $S^z_{\text{tot}} = 1$, the former corresponds to a flip of a single spin out of the xy plane while the latter is related to the breaking of a two-site singlet composing the resonant-valence-bond GS similar to the one of the spin-1 chain exactly solved by Affleck, Kennedy, Lieb and Tasaki [43]. Finally, by decreasing further the value of D, we pass in the Néel phase where both positional and magnetic degrees of freedom orders are signalled by a nonvanishing (spontaneous) magnetization along z

$$M_z^2 \equiv \lim_{R \to \infty} \mathcal{C}_z(R).$$

At the same time $\mathcal{O}_z \neq 0$ but $\mathcal{O}_{x,y} = 0$. Den Nijs and Rommelse ([38], Sect. IIE) introduced yet another less-familiar string correlation function without

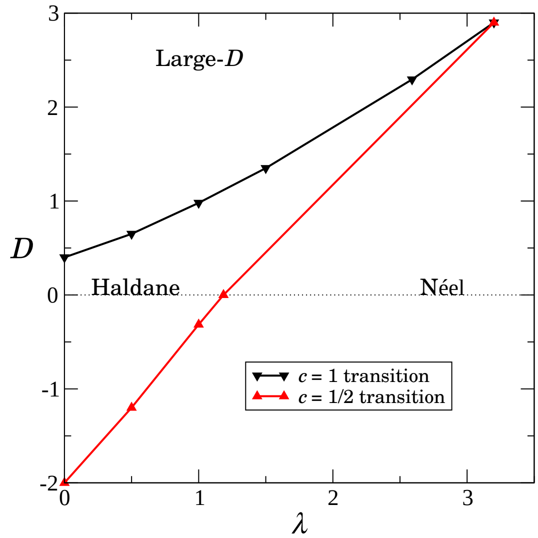

Figure 3.1: Ground-state phase diagram for the model (3.2) in the AFM region $\lambda \geq 0$. The three phases are defined in the text.

spins at the ends

$$G_H(R) \equiv \langle \mathrm{e}^{\mathrm{i}\pi \sum_{j=i}^{i+R} S_j^z} \rangle$$

and argued that $G_H(\infty) = 0$ in the Haldane phase but $G_H(\infty) \neq 0$ in the Large-D and Néel ones.

Hence we may select, equivalently, the pairs $(\mathcal{O}_z, \mathcal{O}_x)$ or $(\mathcal{O}_z, M_z)$ as order parameters to classify the three types of behaviour. The universality classes associated with the two transition lines will be frequently denoted using the language of conformal field theory (CFT - see, for instance, [51, 54, 56]), in particular by specifying the central charge c. We interpret the fully-disordered large-D phase with $(\mathcal{O}_z = 0, \mathcal{O}_x = 0)$ and $(\mathcal{O}_z = 0, M_z = 0)$ as a spin gas. By crossing the $c = 1$ line we enter the Haldane phase where the effective spin-1/2 experience a first magnetic ordering: $(\mathcal{O}_z \neq 0, \mathcal{O}_x \neq 0)$ and $(\mathcal{O}_z \neq 0, M_z = 0)$. Then, loosely speaking, at the $c = 1/2$ line the spin liquid crystallizes and the fully-ordered Néel phase can be interpreted as a spin solid with $(\mathcal{O}_z \neq 0, \mathcal{O}_x = 0)$ and $(\mathcal{O}_z \neq 0, M_z \neq 0)$. Note the interchanged role of $\mathcal{O}_x$ and M_z (see below). In the Néel and Haldane phases $G_H(\infty)$ refers to the positional order of nonzero spins [38], so that it vanishes in the Haldane phase but $G_H(\infty) \neq 0$ in the Néel one.

Phase	$\mathcal{O}_z(R)$	$G_H(R)$
Haldane	Expon. to $\neq 0$	Expon. to 0
Néel	Expon. to $\neq 0$	Expon. to $\neq 0$

Table 3.1: Decay laws of string correlation functions defined in the text, according to Sect. IIE of ref. [38]. To be compared with the results of this chapter, including the explicit form of the algebraic prefactors, as reported in table 3.3.

In order to determine the SOP numerically one has to extrapolate to the thermodynamic limit and to infinite distance the data computed on necessarily finite samples. However, apart from the qualitative statements made in ref. [38] about the exponential decay of the string correlation functions (as reported in table 3.1), the available literature contains scarce information about the spatial behaviour of such correlators and the extrapolation may become problematic, especially close to the transition lines where the bulk correlation length becomes very large. In a particular case, namely the transition from the Large-D to the Haldane phase, the low-energy physics is described by a compactified free boson field theory ($c = 1$ CFT). Once the compactification radius is known in some other independent way, one can read off the decay exponent of the string correlation functions from the set of scaling dimensions of the possible vertex operators. Interestingly, it turns out [57, 58] that, even if the lattice model has periodic boundary conditions (PBC), the vertex operators to be associated with string correlators belong to the sector with *antiperiodic* boundary conditions.

The main purpose of this thesis, instead, is to address the spatial behaviour of spin-spin and string correlation functions in the Haldane and Néel phases, making use of a solvable theory of spinless fermions. Starting from well inside the Néel phase, where the density of sites with $S_i^z = 0$ is negligible, we approximate the problem by assuming that the hidden magnetic order is frozen so that a given contribution to the GS wavefunction can be described by occupation numbers: no fermions if $S_i^z = 0$ and one fermion when $|S_i^z| = 1$, no matter the orientation, which is dictated by the underlying string order. The details of this approach will be presented in Sect.

3.2; actually it is very close to what done by Gómez-Santos in ref. [59]. The difference here is that we include also the single-ion anisotropy term and, in fact, the two formulations are related by a particle-hole transformation. The novelty is that we work out in detail the mapping of the spin-spin and string correlation functions (Sect. 3.3) onto fermionic correlators, so that we can derive in Sect. 3.4 the precise form of their asymptotic behaviour at large distances by exploiting the machinery of Toeplitz determinants. In Sect. 3.5 we generalize the λ-D hamiltonian including a biquadratic interaction: using the same approach we find out that our approximate result for the SOP is the same as the one obtained exactly in [42]. Sect. 3.6 reports a comparison with DMRG simulations of the system in equation (3.2).

3.2 Mapping onto spinless fermions

The basic idea underlying the approximation used is the spin solid picture of the Néel state(s):

$$|N\rangle = |\uparrow\downarrow\uparrow\cdots\downarrow\uparrow\downarrow\cdots\uparrow\downarrow\rangle \tag{3.3}$$

which is, in fact, the GS of the Hamiltonian (3.2) for $\lambda \to \infty$ at fixed D or $D \to -\infty$ and $\lambda > 0$. Actually the GS is doubly degenerate: for a given configuration of the type (3.3) with, say, $S_i^z = 1$ at the reference site $i = 0$, the energy is unchanged by the Z_2 transformation $T = \exp(\mathrm{i}\pi \sum_j S_j^y)$ that performs a π-rotation about the y-axis (spin-flip). We will refer to $|N\rangle$ and $|\bar{N}\rangle = T|N\rangle$ as Néel and anti-Néel states, respectively. Now, in a perturbative fashion, when $|D|$ and/or $\lambda \gg 1$ the effect of the transverse terms in the Hamiltonian $S_i^{x,y}S_{i+1}^{x,y}$ is to:

i) create pairs of adjacent sites with $S_i^z = S_{i+1}^z = 0 : |\uparrow\downarrow\rangle \to |0\,0\rangle$;

ii) move the zeroes in the AFM background, e.g.: $|\uparrow 0\rangle \to |0\uparrow\rangle$;

iii) re-create a pair $\uparrow\downarrow$ or $\downarrow\uparrow$ in place of a pair of adjacent zeroes.

Notice that ii) preserves the AFM order, albeit not on nearest neighbours but mediated by string of zeroes (hidden order). Again, due to the AFM order (induced by $\lambda > 0$ and by the transverse terms), even if both states of iii) can be created in an "island" of zeroes, as far as the low-energy part of the spectrum is concerned, one of the two will be preferred according to the orientation of the surrounding spins, that is, by the hidden AFM order. Note also that $|N\rangle$ and $|\bar{N}\rangle$ are connected through a large number of virtual processes, so that in the thermodynamic limit only one of the two will be selected by a spontaneous symmetry breaking mechanism induced by an infinitesimal staggered magnetic field. Alternatively, if the system under consideration is described by a thermal density matrix $\exp(-\beta H)$, when $\beta \to \infty$ the GS reduces to a symmetric mixed state $|N\rangle\langle N| + |\bar{N}\rangle\langle\bar{N}|$.

Once the question of the GS is accounted for, from the scenario above one can see that the orientation of spins with nonzero component along z is determined by the hidden order and can be taken for granted. The validity of such an approximation is ultimately measured by the values of the longitudinal SOP: the closer is $\mathcal{O}_z$ to unity the higher is the AFM order of nonzero spins. We then introduce the following fermionic picture: assign a spinless fermion $|+_i\rangle \equiv c_i^\dagger|-_i\rangle$ at site i if $S_i^z \neq 0$ and no fermions $|-_i\rangle \equiv |0_i\rangle$ in the spin language if $S_i^z = 0$. (This notation for spinless fermions has a direct translation in the language of the XY model that will be introduced at the end of this section.) Process ii) is nothing but a hopping of spinless fermions, while processes i) and iii) represent annihilation and creation of pairs $|+_i +_{i+1}\rangle$. The density of nonzero spins $(S_i^z)^2$ is simply translated to the local fermion number $n_i = c_i^\dagger c_i$, while, due to the underlying AFM order, the Ising-like term takes the form $-\lambda n_i n_{i+1}$ that contributes with a negative energy when two fermions are present on adjacent sites.

Hence, under the hypothesis of hidden AFM order, the dynamics of equation (3.2) is reproduced by the following effective fermionic model

$$\mathcal{H}_{\mathrm{f}} = \sum_j \left(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j + c_j^\dagger c_{j+1}^\dagger + c_{j+1} c_j - \lambda n_j n_{j+1} + D n_j \right) \tag{3.4}$$

(acting in a reduced Hilbert space $\mathcal{H} = \otimes_i \mathcal{H}_i^{(2)}$where $\mathcal{H}^{(2)}$ denotes the local Hilbert space of a two-level system - as that of a spinless fermion or a spin-1/2 introduced below). It should be observed that equation (3.4) with $D = 0$ is essentially equivalent (apart from an additive constant) to equation (2) of ref. [59] once a particle-hole transformation $n_i \to 1 - n_i$ is performed at every site.

Following Gómez-Santos [59] we now proceed to a further approximation on the fermionic Hamiltonian that is not amenable to an exact treatment due to the λ-term. At the Hartree-Fock level this term can be approximated as:

$$n_j n_{j+1} \simeq (n_j + n_{j+1}) \langle n_j \rangle - \left(c_j^\dagger c_{j+1} \langle c_{j+1}^\dagger c_j \rangle + \text{h.c.} \right) + \left(c_j^\dagger c_{j+1}^\dagger \langle c_{j+1} c_j \rangle + \text{h.c.} \right)$$
$$- \left(\langle n_j \rangle^2 - \langle c_{j+1}^\dagger c_j \rangle \langle c_j^\dagger c_{j+1} \rangle + \langle c_{j+1} c_j \rangle \langle c_j^\dagger c_{j+1}^\dagger \rangle \right)$$

where the expectation values $\langle \dots \rangle$ now are taken with respect to the GS of the quadratic Hamiltonian

$$\mathcal{H}_{\text{HF}} = \sum_j \Big[(1 + \lambda A)\, c_j^\dagger c_{j+1} + (1 - \lambda B)\, c_j^\dagger c_{j+1}^\dagger + \text{h.c.} \Big]$$
$$+ (D - 2\lambda n_0)\, n_j + \lambda \left(n_0^2 - |A|^2 + |B|^2 \right) \tag{3.5}$$

where the parameters

$$n_0 \equiv \langle n_j \rangle \ , \quad A \equiv \langle c_{j+1}^\dagger c_j \rangle \ , \quad B = \langle c_{j+1} c_j \rangle$$

have to be determined self-consistently. The advantage of a Hamiltonian of the form (3.5) is that it can be diagonalized by means of a Bogoliubov transformation

$$\eta_k = \cos \frac{\theta_k}{2} c_k + \mathrm{i} \sin \frac{\theta_k}{2} c_{-k}^\dagger$$

where $c_k = 1/\sqrt{L} \sum_j c_j \exp(-\mathrm{i} jk)$ and θ_k is given by

$$e^{\mathrm{i}\theta_k} = \frac{(\cos k - h + \mathrm{i}\gamma \sin k)}{\Lambda_k}$$

where

$$h \equiv \frac{2\lambda n_0 - D}{2\,(1 + \lambda A)} \ , \quad \gamma \equiv \frac{1 - \lambda B}{1 + \lambda A} \tag{3.6}$$
$$\Lambda_k = \sqrt{(\cos k - h)^2 + \gamma^2 \sin k^2}$$

Note that, as we are interested in the thermodynamic limit, we do not specify here the boundary conditions on the spin and fermionic Hamiltonians. The momenta are quantized as $\Delta k = 2\pi/L$ and their precise location within the first Brillouin zone depend on the conditions imposed on the end sites. However, for $L \to \infty$

$$\frac{1}{L}\sum_k \to \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}k.$$

Apart from additive terms of $O(L^{-1})$ the Hamiltonian in diagonal form is

$$\mathcal{H}_{\mathrm{HF}} = 2(1+\lambda A)\sum_k \Lambda_k \left(\eta_k^\dagger \eta_k - \frac{1}{2}\right) + U$$

and $U = (D - 2\lambda n_0)/2 + \lambda(n_0^2 - A^2 + B^2)$. In the thermodynamic limit, the self-consistency equations are

$$n_0 = \frac{1}{2} - \frac{1}{2\pi}\int_0^\pi dk \frac{-h\,(n_0, A) + \cos k}{\Lambda(k)} \tag{3.7}$$

$$A = -\frac{1}{2\pi}\int_0^\pi dk \frac{(-h\,(n_0, A) + \cos k)\cos k}{\Lambda(k)} \tag{3.8}$$

$$B = -\frac{1}{2\pi}\int_0^\pi dk \frac{\gamma\,(A, B)\sin^2 k}{\Lambda(k)}. \tag{3.9}$$

The notation used in equation (3.6) is the one commonly used for the XY spin-1/2 model in a transverse field (see Section 1.2). In fact, by (inverse) Jordan-Wigner transform one gets [56]

$$\mathcal{H}_{\mathrm{HF}} \to \mathcal{H}_{\mathrm{XY}} = \sum_j \left(\frac{1+\gamma}{2}\right)\sigma_j^x \sigma_{j+1}^x + \left(\frac{1-\gamma}{2}\right)\sigma_j^y \sigma_{j+1}^y - h\sigma_j^z \tag{3.10}$$

where the σ_j^α's are Pauli matrices at site j. This model is known [56] to be critical at $h = \pm 1$ for $\gamma \neq 0$, where it belongs to the $c = 1/2$ universality class (the same as the 2D classical Ising model) and at $\gamma = 0$ for $h \in (-1, 1)$ where the universality class becomes that of the compactified free boson, $c = 1$.

From the numerical solutions of (3.7)-(3.9) it turns out that in the Haldane and Néel phases $A < 0$ and $B < 0$ so that $\gamma > 1$ (as long as $\lambda|A| < 1$ - some representative cases are listed in table 3.2), while most studies are limited to $|\gamma| < 1$. As a consequence the region $\gamma^2 < 1 - h^2$ corresponding to oscillations with wavenumber different from π [11], [56] is not present in our case. However, having $\gamma > 1$ does not affect the critical condition we are interested in, that remains $h = \pm 1$. In these cases we have just $c = 1/2$, as reported before [54] for the Haldane-to-Néel transition. At $\lambda = 0$, $D \cong -2$

this transition line merges with the boundary towards the so-called XY phases corresponding to $c = 1$. Interestingly this change of universality class is captured also by our approximation since for $\lambda = 0$, $D = -2$ the self-consistent solution yields just $\gamma = 1$ and $h = 1$. From the data in table 3.2 one can also estimate, for example, the critical value of D at fixed $\lambda = 1$; the result is $D_{\mathrm{c}} \cong -0.214$, which is not in good quantitative agreement with the numerical value $D_{\mathrm{c}} = -0.315$ [54, 58]. The perturbation of the isotropic Heisenberg Hamiltonian with $\lambda > 1$ and $D = 0$, instead, seems to be better described by the spinless fermions approach; already at this level of approximation the value $\lambda_{\mathrm{c}} = 1.125$ found in [59] is close to the best DMRG independent estimate $\lambda_{\mathrm{c}} = 1.1856$ [61]. Even if it is likely that the inclusion of configurations with nearest-neighbour parallel spins could improve the results, as discussed by Gómez-Santos [59], we do not insist along this line here because we are ultimately interested in the decay laws of correlation functions that are essentially dictated by the universality classes. In fact, it is important to stress that neither the extension to $D \neq 0$, nor the extension of the model as in equation (8) of ref. [59] modify the universality class of the transition, that remains of the $c = 1/2$ (or Ising) type for $\lambda > 0$. Although the location of the critical points and of the prefactors depend on the values of the parameters, the scaling dimensions of the operators in the continuum field theory (i.e. the decay exponents of the correlation functions) do not change when we move along the $c = 1/2$ line. Nonetheless, due to the lack of an explicit mapping of the spin-1 strings onto the corresponding correlators in the Ising fermionic field theory, up to now the exponents appearing in the large-distance decay of string correlation functions were unknown. This is precisely the subject of subsecs. 3.4.1 and 3.4.3. Eventually, we note that alternative pictures of the Haldane gap in fermionic language can be derived by perturbation theory near the Babujian-Takhtajan integrable biquadratic spin-1 chain [62] or from two-leg ladders with ferromagnetic coupling on the rungs [63].

At this stage it is interesting to compare the entanglement properties of the original spin-1 model (eq. (3.2)) with those of the XY spin-1/2 chain resulting from the mapping. On the one hand, for the former it has been shown [64] that at the isotropic Heisenberg point $\lambda = 1$, $D = 0$ there is long-

λ	D	n_0	A	B	h	γ
1	0	0.709	−0.158	−0.253	0.842	1.49
1	−0.125	0.745	−0.137	−0.246	0.936	1.44
1	−0.200	0.774	−0.117	−0.240	0.990	1.41
1	−0.250	0.800	−0.0979	−0.235	1.03	1.37
1	−0.300	0.816	−0.0866	−0.231	1.06	1.35
1	−0.315	0.820	−0.0837	−0.230	1.07	1.34
1	−0.330	0.824	−0.0811	−0.229	1.08	1.34
1	−0.345	0.828	−0.0786	−0.228	1.09	1.33
1	−0.400	0.841	−0.0706	−0.223	1.12	1.32
1	−0.450	0.850	−0.0645	−0.219	1.15	1.30
1	−0.750	0.893	−0.0406	−0.198	1.32	1.25
1	−0.875	0.904	−0.0344	−0.190	1.39	1.23
1	−10	0.996	−0.000317	−0.0433	6.00	1.04
5	−0.125	0.991	−0.000853	−0.0649	5.04	1.33

Table 3.2: Self-consistent estimates of the three decoupling parameters n_0, A and B of equations (3.7)-(3.9) for some choices of λ and D in the Haldane and Néel phases. It must be kept in mind that the continuum versions of the self-consistent equations neglect some $O(L^{-1})$ terms coming from isolated contributions at wavenumber 0 or π. Last two column contain the corresponding parameters h and γ of the effective XY model according to equation (3.6).

distance spin-1 (qutrit) entanglement in the thermodynamic limit for two sites arbitrarily far apart. It is reasonable to expect that this entanglement survives in a neighbourhood of the isotropic point. On the other hand, in ref. [65] it is stated that the qubit entanglement in the XY model with transverse field vanishes beyond a distance of order γ^{-1}. In our case $\gamma > 1$ and the degrees of freedom of the qubits represent the presence or the absence of an effective particle with $|S_i^z| = 1$. Therefore we are led to speculate that wherever there is full spin-1 entanglement in the vicinity of the Heisenberg point, this is due to the spin correlations between the sites with $S_i^z \neq 0$. Recalling the hypothesis of underlying string order and imagining to eliminate the sites with $S_i^z = 0$, the qualitative picture of the long-distance entangled states in the Haldane region if that of a Greenberger-Horne-Zeilinger state [66] with effective AFM order $|\ldots\uparrow\downarrow\uparrow\downarrow\ldots\rangle + |\ldots\downarrow\uparrow\downarrow\uparrow\ldots\rangle$.

3.3 Mapping for the spin-spin and string correlators

3.3.1 Mapping for the longitudinal correlator $\mathcal{C}_z$

We shall exploit now the mapping from spin-1 to spinless fermions, based on the existence of an underlying string order, to translate the various spin-1 correlation functions onto expectation values of strings of fermionic operators that can be computed exactly when the Hamiltonian has the form (3.5). Let us start from the z-component of the spin [60]

$$S_j^z \to n_j K_j \to \frac{1+\sigma_j^z}{2} K_j \tag{3.11}$$

where $K_j = \exp(\mathrm{i}\pi \sum_{i<j} n_i) = \prod_{i<j}(-\sigma_i^z)$ is a Jordan-Wigner tail that accounts for the correct sign when $S_j^z \neq 0$ assuming, conventionally, that the first nonzero spin is pointing up (we get a $-$ sign if instead we assume that the first non-zero spin is pointing down). By inserting the expression $S_j^z = \frac{1+\sigma_j^z}{2} \prod_{i<j}(-\sigma_j^z)$ into the definition of the longitudinal spin-spin correlation function and using the properties of Pauli matrices one finds [60]

$$\mathcal{C}_z(R) \to \frac{1}{4}(-1)^R \langle \left(1+\sigma_j^z\right) \prod_{k<j} (-\sigma_k^z) \prod_{k<j+R} (-\sigma_k^z) \left(1+\sigma_{j+R}^z\right) \rangle$$

$$= \frac{1}{4} \left(\langle \prod_{k=j}^{j+R} \sigma_k^z \rangle + \langle \prod_{k=j+1}^{j+R} \sigma_k^z \rangle + \langle \prod_{k=j}^{j+R-1} \sigma_k^z \rangle + \langle \prod_{k=j+1}^{j+R-1} \sigma_k^z \rangle \right). \tag{3.12}$$

3.3.2 Mapping for the transverse correlator $\mathcal{C}_x$

Let's consider now the transverse correlation function

$$\mathcal{C}_x(R) = \frac{1}{2} \langle \left(S_j^+ S_{j+R}^- + S_j^- S_{j+R}^+ \right) \rangle \tag{3.13}$$

and see how it can be translated onto fermions. Let's consider the action of $\mathcal{C}_x$ on a state with an even number of zero spins between j and $j+R$.

- There are non zero spins both in j and $j+R$

$$\mathcal{C}_x |\cdots 0 \uparrow 0 \cdots 0 \downarrow_j 0 \cdots 0 \uparrow 0 \cdots 0 \downarrow 0 \cdots 0 \uparrow_{j+R} 0 \cdots 0 \downarrow 0 \cdots \rangle =$$

$$|\cdots 0 \uparrow 0 \cdots 0 0_j 0 \cdots 0 \uparrow 0 \cdots 0 \downarrow 0 \cdots 0 0_{j+R} 0 \cdots 0 \downarrow 0 \cdots \rangle \tag{3.14}$$

- There is a non zero spin in j or $j+R$

$$\mathcal{C}_x |\cdots 0 \uparrow 0 \cdots 0 0_j 0 \cdots 0 \downarrow 0 \cdots 0 \uparrow 0 \cdots 0 \downarrow_{j+R} 0 \cdots 0 \uparrow 0 \cdots \rangle =$$

$$|\cdots 0 \uparrow 0 \cdots 0 \uparrow_j 0 \cdots 0 \downarrow 0 \cdots 0 \uparrow 0 \cdots 0 0_{j+R} 0 \cdots 0 \uparrow 0 \cdots \rangle \tag{3.15}$$

- There are zero spins both in j and $j+R$

$$\mathcal{C}_x |\cdots 0 \uparrow 0 \cdots 0 0_j 0 \cdots 0 \downarrow 0 \cdots 0 \uparrow 0 \cdots 0 0_{j+R} 0 \cdots 0 \downarrow 0 \cdots \rangle =$$

$$|\cdots 0 \uparrow 0 \cdots 0 \uparrow_j 0 \cdots 0 \downarrow 0 \cdots 0 \uparrow 0 \cdots 0 \downarrow_{j+R} 0 \cdots 0 \downarrow 0 \cdots \rangle +$$

$$|\cdots 0 \uparrow 0 \cdots 0 \downarrow_j 0 \cdots 0 \downarrow 0 \cdots 0 \uparrow 0 \cdots 0 \uparrow_{j+R} 0 \cdots 0 \downarrow 0 \cdots \rangle \tag{3.16}$$

In all cases the hidden order does not hold anymore. Consider now states with an odd number of non-zero spins between j and $j+R$.

- There are non zero spins both in j and $j+R$

$$\mathcal{C}_x|\cdots 0\uparrow 0\cdots 0\downarrow_j 0\cdots 0\uparrow 0\cdots 0\downarrow_{j+R} 0\cdots 0\uparrow 0\cdots\rangle = 0 \quad (3.17)$$

- There is a non zero spin in j or $j+R$

$$\mathcal{C}_x|\cdots 0\uparrow 0\cdots 0\downarrow_j 0\cdots 0\uparrow 0\cdots 00_{j+R}0\cdots 0\downarrow 0\cdots\rangle =$$

$$|\cdots 0\uparrow 0\cdots 00_j0\cdots 0\uparrow 0\cdots 0\downarrow_{j+R} 0\cdots 0\downarrow 0\cdots\rangle \quad (3.18)$$

- There are zero spins both in j and $j+R$

$$\mathcal{C}_x|\cdots 0\uparrow 0\cdots 00_j0\cdots 0\downarrow 0\cdots 00_{j+R}0\cdots 0\uparrow 0\cdots\rangle =$$

$$|\cdots 0\uparrow 0\cdots 0\uparrow_j 0\cdots 0\downarrow 0\cdots 0\downarrow_{j+R} 0\cdots 0\uparrow 0\cdots\rangle +$$

$$|\cdots 0\uparrow 0\cdots 0\downarrow_j 0\cdots 0\downarrow 0\cdots 0\uparrow_{j+R} 0\cdots 0\uparrow 0\cdots\rangle \quad (3.19)$$

These cases do not preserve the hidden order too; from these remarks we see that the only configurations which preserve the hidden order are those with no non zero spins between sites j and $j+R$. Let's consider now states with no non zero spins between j and $j+R$

- There are non zero spins both in j and $j+R$

$$\mathcal{C}_x|\cdots 0\uparrow 0\cdots 0\downarrow_j 0\cdots 0\uparrow_{j+R} 0\cdots 0\downarrow 0\cdots\rangle =$$

$$|\cdots 0\uparrow 0\cdots 00_j0\cdots 00_{j+R}0\cdots 0\downarrow 0\cdots\rangle \quad (3.20)$$

- There is a non zero spin in j or $j+R$

$$\mathcal{C}_x|\cdots 0\uparrow 0\cdots 0\downarrow_j 0\cdots 00_{j+R}0\cdots 0\uparrow 0\cdots\rangle =$$

$$|\cdots 0\uparrow 0\cdots 00_j0\cdots 0\downarrow_{j+R} 0\cdots 0\uparrow 0\cdots\rangle \quad (3.21)$$

- There are zero spins both in j and $j+R$

$$\mathcal{C}_x|\cdots 0\uparrow 0\cdots 00_j 0\cdots 00_{j+R}0\cdots 0\downarrow 0\cdots\rangle =$$

$$|\cdots 0\uparrow 0\cdots 0\uparrow_j 0\cdots 0\downarrow_{j+R} 0\cdots 0\downarrow 0\cdots\rangle +$$

$$|\cdots 0\uparrow 0\cdots 0\downarrow_j 0\cdots 0\uparrow_{j+R} 0\cdots 0\downarrow 0\cdots\rangle \tag{3.22}$$

We notice that all these configurations, except the first one[1] in (3.22), preserve the string order. We see then that the identification [60]

$$\mathcal{C}_x(R) = \frac{1}{2}\left(S_j^+ S_{j+R}^- + S_j^- S_{j+R}^+\right) \to \sigma_j^x \prod_{k=j+1}^{j+R-1}\left(\frac{1-\sigma_k^z}{2}\right)\sigma_{j+R}^x \tag{3.23}$$

has the correct action, since the only cases in which the l.h.s. does not break the string order are those with $S_k^z = 0$, that is $\sigma_k^z = -1$, on all sites between j and $j+R$. The product on the r.h.s. of (3.23) is exactly the expression involved in the so-called emptiness formation probability (see, for example, [67] and refs. therein).

3.3.3 Mapping for the longitudinal string $\mathcal{O}_z$

Let us study now the spin-1 strings. Along the z-direction we have simply

$$e^{i\pi\sum_{k<j} S_k^z} = \prod_{k<j}\left(1-2(S_k^z)^2\right) \to \prod_{k<j}(-\sigma_k^z)\,. \tag{3.24}$$

Again by using the relation $S_j^z = \frac{1+\sigma_j^z}{2}\prod_{i<j}(-\sigma_j^z)$ and plugging the string written above into eq. (3.1) one gets [60]

$$\mathcal{O}_z(R) \to \left\langle \left(\frac{1+\sigma_j^z}{2}\right)\prod_{k<j}(-\sigma_k^z)\prod_{k=j+1}^{j+R-1}(-\sigma_k^z)\prod_{k<j+R}(-\sigma_k^z)\left(\frac{1+\sigma_{j+R}^z}{2}\right)\right\rangle$$

$$= -\langle\left(\frac{1+\sigma_j^z}{2}\right)\left(\frac{1+\sigma_{j+R}^z}{2}\right)\rangle = -\frac{1}{4}\left(1+\langle\sigma_j^z\rangle+\langle\sigma_{j+R}^z\rangle+\langle\sigma_j^z\sigma_{j+R}^z\rangle\right) \tag{3.25}$$

[1] This configuration gives no contribution to the expectation value

Note that in the language of the effective XY model, the Néel correlation function (3.12) involves a string of Pauli operators whereas the string correlation function (3.25) involves only one- and two-points correlators of the σ's. Thanks to equation (3.24) we easily obtain also the pure-string correlation function as:

$$G_H(R) \to (-1)^{R+1} \left\langle \prod_{j=i}^{i+R} \sigma_j^z \right\rangle . \tag{3.26}$$

From equation (3.12) we see that, in this approach, $G_H(R)$ is nothing but the first term of the usual spin-spin correlation function $\mathcal{C}_z(R)$ apart from the prefactor.

3.3.4 Mapping for the transverse string $\mathcal{O}_x$

We finally consider the string operator along the x direction $\mathcal{O}_x$. First of all, we notice that fact that

$$\mathrm{e}^{\mathrm{i}\pi S^x} = \begin{pmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{pmatrix}$$

that is, apart from an overall sign, the operator above performs a swap between $S_j^z = 1$ and $S_j^z = -1$ leaving the $S_j^z = 0$ component isolated.

We define now the operators

$$\mathcal{P}_{\pm,j} = \frac{1}{2}\left[1 \mp \prod_{k<j}(-\sigma_k^z)\right] \tag{3.27}$$

as the operator that ensures us that the last non zero spin before site j is pointing up (down), and

$$\mathcal{Q}_{\pm,i}^j = \frac{1}{2}\left[1 \pm \prod_{k=i}^{j}(-\sigma_k^z)\right] \tag{3.28}$$

as the projector onto states with an even (odd) number of non zero spins between i and j.

Let's consider first configurations with an even number of non zero spins between j and $j + R$

- There are non zero spins both in j and $j+R$

$$\hat{\mathcal{O}}_x|\cdots 0\cdots 0\uparrow 0\cdots 0\downarrow_j 0\cdots 0\uparrow 0\cdots 0\downarrow 0\cdots 0\uparrow_{j+R} 0\cdots 0\downarrow 0\cdots\rangle \rightarrow$$

$$|\cdots 0\cdots 0\uparrow 0\cdots 00_j 0\cdots 0\downarrow 0\cdots 0\uparrow 0\cdots 00_{j+R} 0\cdots 0\downarrow 0\cdots\rangle \quad (3.29)$$

that preserves the string order. The correct action of the string operator $\hat{\mathcal{O}}_x$ in terms of the spin 1/2 operators is given by

$$\hat{\mathcal{O}}_x \propto \mathcal{P}_{+,j}\sigma_j^- \mathcal{Q}_{+,j}^{j+R}\sigma_{j+R}^-$$

If we consider instead the state with a spin pointing up in j and a spin pointing down in $j+R$, analogous to the one treated above, we have

$$\hat{\mathcal{O}}_x \propto \mathcal{P}_{-,j}\sigma_j^- \mathcal{Q}_{+,j}^{j+R}\sigma_{j+R}^-$$

Collecting terms we have

$$\hat{\mathcal{O}}_x \propto \sigma_j^- \mathcal{Q}_{+,j}^{j+R}\sigma_{j+R}^- \quad (3.30)$$

- There is a spin $\downarrow$ in j and a spin 0 in $j+R$

$$\hat{\mathcal{O}}_x|\cdots 0\cdots 0\uparrow 0\cdots 0\downarrow_j 0\cdots 0\uparrow 0\cdots 0\downarrow 0\cdots 00_{j+R} 0\cdots 0\uparrow 0\cdots\rangle \rightarrow$$

$$\left[\begin{array}{l} |\cdots 0\cdots 0\uparrow 0\cdots 00_j 0\cdots 0\downarrow 0\cdots 0\uparrow 0\cdots 0\downarrow_{j+R} 0\cdots 0\uparrow 0\cdots\rangle \\ |\cdots 0\cdots 0\uparrow 0\cdots 00_j 0\cdots 0\downarrow 0\cdots 0\uparrow 0\cdots 0\uparrow_{j+R} 0\cdots 0\uparrow 0\cdots\rangle \end{array}\right. \quad (3.31)$$

We see that the first configuration preserves the hidden order, while the second one breaks it. The string operator becomes

$$\hat{\mathcal{O}}_x \propto \sigma_j^- \mathcal{Q}_{+,j}^{j+R}\mathcal{P}_{+,j+R}\sigma_{j+R}^+$$

$P_{+,j+R}$ guarantees that the last non zero spin before $j+R$ is pointing up, ensuring thus that in the spin 1/2 picture the spin is created with the "correct" orientation. Proceeding as in the previous case, we have

$$\mathcal{O}_x \propto \sigma_j^- \mathcal{Q}_{+,j}^{j+R}\sigma_{j+R}^+ \quad (3.32)$$

- There is a spin 0 in j and a spin $\downarrow$ in $j+R$

$$\hat{\mathcal{O}}_x|\cdots 0\cdots 0\uparrow 0\cdots 00_j 0\cdots 0\downarrow 0\cdots 0\uparrow 0\cdots 0\downarrow_{j+R} 0\cdots 0\uparrow 0\cdots\rangle \rightarrow$$

$$\left[\begin{array}{l} |\cdots 0\cdots 0\uparrow 0\cdots 0\downarrow_j 0\cdots 0\uparrow 0\cdots 0\downarrow 0\cdots 00_{j+R} 0\cdots 0\uparrow 0\cdots\rangle \\ |\cdots 0\cdots 0\uparrow 0\cdots 0\uparrow_j 0\cdots 0\uparrow 0\cdots 0\downarrow 0\cdots 00_{j+R} 0\cdots 0\uparrow 0\cdots\rangle \end{array}\right. \tag{3.33}$$

Again, the state on the first line still preserves the hidden antiferromagnetic order, while the second doesn't. The correct action for the string operator is

$$\hat{\mathcal{O}}_x \propto \mathcal{P}_{+,j}\sigma_j^+ \mathcal{Q}_{+,j}^{j+R}\sigma_{j+R}^-$$

and so, as in the previous cases

$$\hat{\mathcal{O}}_x \propto \sigma_j^+ \mathcal{Q}_{+,j}^{j+R}\sigma_{j+R}^- \tag{3.34}$$

- Finally, let's consider a state with spin 0 both in j and $j+R$

$$\hat{\mathcal{O}}_x|\cdots 0\cdots 0\uparrow 0\cdots 00_j 0\cdots 0\downarrow 0\cdots 0\uparrow 0\cdots 00_{j+R} 0\cdots 0\downarrow 0\cdots\rangle \rightarrow$$

$$\left[\begin{array}{l} |\cdots 0\cdots 0\uparrow 0\cdots 0\downarrow_j 0\cdots 0\uparrow 0\cdots 0\downarrow 0\cdots 0\uparrow_{j+R} 0\cdots 0\downarrow 0\cdots\rangle \\ |\cdots 0\cdots 0\uparrow 0\cdots 0\downarrow_j 0\cdots 0\uparrow 0\cdots 0\downarrow 0\cdots 0\downarrow_{j+R} 0\cdots 0\downarrow 0\cdots\rangle \\ |\cdots 0\cdots 0\uparrow 0\cdots 0\uparrow_j 0\cdots 0\uparrow 0\cdots 0\downarrow 0\cdots 0\uparrow_{j+R} 0\cdots 0\downarrow 0\cdots\rangle \\ |\cdots 0\cdots 0\uparrow 0\cdots 0\uparrow_j 0\cdots 0\uparrow 0\cdots 0\downarrow 0\cdots 0\downarrow_{j+R} 0\cdots 0\downarrow 0\cdots\rangle \end{array}\right. \tag{3.35}$$

The first state still has string order, while the other three configurations break the order. We have

$$\hat{\mathcal{O}}_x \propto \mathcal{P}_{+,j}\frac{1+\sigma_j^z}{2}\prod_{k<j}(-\sigma_k^z)\sigma_j^+ \mathcal{Q}_{+,j}^{j+R}\sigma_{j+R}^+$$

and considering also the state with the last non zero spin before j pointing down, we have

$$\hat{\mathcal{O}}_x \propto \sigma_j^z \mathcal{Q}_{+,j}^{j+R}\sigma_{j+R}^+ \tag{3.36}$$

We find then, that the action of $\hat{\mathcal{O}}_x$ on states with string order and an even number of non zero spin between j and $j+R$ gives rise to only one configuration that still respects the hidden antiferromagnetic order, contributing thus to the expectation value

$$\mathcal{O}_x = \langle S_j^x e^{i\pi \sum_{k=j+1}^{j+R-1} S_k^x} S_{j+R}^x \rangle$$

while producing some other configurations that do not respect the hidden order. Collecting the terms obtained

$$\hat{\mathcal{O}}_x \propto \sigma_j^x \mathcal{Q}_{+,j}^{j+R} \sigma_{j+R}^x = \sigma_j^x \left[\frac{1 + \prod_{k=j+1}^{j+R-1}(-\sigma_k^z)}{2} \right] \sigma_{j+R}^x \tag{3.37}$$

The configurations with an odd number of states between the two reference sites are treated exactly in the same way.

- There are non zero spins both in j and $j+R$

$$\hat{\mathcal{O}}_x | \cdots 0 \cdots 0 \uparrow 0 \cdots 0 \downarrow_j 0 \cdots 0 \uparrow 0 \cdots 0 \downarrow_{j+R} 0 \cdots 0 \uparrow 0 \cdots \rangle \rightarrow$$

$$| \cdots 0 \cdots 0 \uparrow 0 \cdots 0 0_j 0 \cdots 0 \downarrow 0 \cdots 0 0_{j+R} 0 \cdots 0 \uparrow 0 \cdots \rangle$$

  that preserves the string order

$$\hat{\mathcal{O}}_x \propto \sigma_j^- \mathcal{Q}_{-,j}^{j+R} \sigma_{j+R}^- \tag{3.38}$$

- There is a non zero spin in j and a spin 0 in $j+R$

$$\hat{\mathcal{O}}_x | \cdots 0 \cdots 0 \uparrow 0 \cdots \downarrow_j 0 \cdots 0 \uparrow 0 \cdots 0 0_{j+R} 0 \cdots 0 \downarrow 0 \cdots 0 \uparrow 0 \cdots \rangle \rightarrow$$

$$\left[\begin{array}{l} | \cdots 0 \cdots 0 \uparrow 0 \cdots 0_j 0 \cdots 0 \downarrow 0 \cdots 0 \uparrow_{j+R} 0 \cdots 0 \downarrow 0 \cdots 0 \uparrow 0 \cdots \rangle \\ | \cdots 0 \cdots 0 \uparrow 0 \cdots 0_j 0 \cdots 0 \downarrow 0 \cdots 0 \downarrow_{j+R} 0 \cdots 0 \downarrow 0 \cdots 0 \uparrow 0 \cdots \rangle \end{array} \right. \tag{3.39}$$

  and just the configuration on the first line keeps the order

$$\hat{\mathcal{O}}_x \propto \sigma_j^- \mathcal{Q}_{-,j}^{j+R} \sigma_{j+R}^+ \tag{3.40}$$

- There is a spin 0 in j and a non zero spin in $j+R$

$$\hat{\mathcal{O}}_x | \cdots 0 \cdots 0 \uparrow 0 \cdots 0 \downarrow \cdots 0 \cdots 0 0_j 0 \cdots 0 \uparrow 0 \cdots 0 \downarrow_{j+R} 0 \cdots 0 \uparrow 0 \cdots \rangle \rightarrow$$

$$\left[\begin{array}{l} | \cdots 0 \cdots 0 \uparrow 0 \cdots 0 \downarrow \cdots 0 \cdots 0 \uparrow_j 0 \cdots 0 \downarrow 0 \cdots 0 0_{j+R} 0 \cdots 0 \uparrow 0 \cdots \rangle \\ | \cdots 0 \cdots 0 \uparrow 0 \cdots 0 \downarrow \cdots 0 \cdots 0 \downarrow_j 0 \cdots 0 \downarrow 0 \cdots 0 0_{j+R} 0 \cdots 0 \uparrow 0 \cdots \rangle \end{array} \right. \tag{3.41}$$

  Just the first of these states preserves the order.

$$\hat{\mathcal{O}}_x \propto \sigma_j^+ \mathcal{Q}_{-,j}^{j+R} \sigma_{j+R}^- \tag{3.42}$$

- Finally there is a spin 0 both in j and $j+R$

$$\mathcal{O}_x|0\cdots 0\uparrow 0\cdots 0\downarrow 0\cdots 00_j 0\cdots 0\uparrow 0\cdots 00_{j+R}0\cdots 0\downarrow 0\cdots 0\uparrow 0\cdots\rangle \rightarrow$$

$$\left[\begin{array}{l} |0\cdots 0\uparrow 0\cdots 0\downarrow 0\cdots 0\uparrow_j 0\cdots 0\downarrow 0\cdots 0\uparrow_{j+R} 0\cdots 0\downarrow 0\cdots 0\uparrow 0\cdots\rangle \\ |0\cdots 0\uparrow 0\cdots 0\downarrow 0\cdots 0\uparrow_j 0\cdots 0\downarrow 0\cdots 0\downarrow_{j+R} 0\cdots 0\downarrow 0\cdots 0\uparrow 0\cdots\rangle \\ |0\cdots 0\uparrow 0\cdots 0\downarrow 0\cdots 0\downarrow_j 0\cdots 0\downarrow 0\cdots 0\uparrow_{j+R} 0\cdots 0\downarrow 0\cdots 0\uparrow 0\cdots\rangle \\ |0\cdots 0\uparrow 0\cdots 0\downarrow 0\cdots 0\downarrow_j 0\cdots 0\downarrow 0\cdots 0\downarrow_{j+R} 0\cdots 0\downarrow 0\cdots 0\uparrow 0\cdots\rangle \end{array}\right. \quad (3.43)$$

The first configuration preserves the order while the other three don't.

$$\hat{\mathcal{O}}_x \propto \sigma^+ \mathcal{Q}_{-,j}^{j+R} \sigma_{j+R}^+ \quad (3.44)$$

We find, as well as in the even case, that every state with string order gives a non zero contribution to the expectation value (3.37). Collecting the terms obtained for these configurations we have

$$\hat{\mathcal{O}}_x \propto -\sigma_j^x \mathcal{Q}_{-,j}^{j+R} \sigma_{j+R}^x = -\sigma_j^x \left[\frac{1 - \prod_{k=j+1}^{j+R-1}(-\sigma_k^z)}{2}\right] \sigma_{j+R}^x \quad (3.45)$$

From (3.37) and (3.45) we have that the transverse string order parameter is given by [60]

$$\mathcal{O}_x = (-1)^{R-1} \frac{\langle \sigma_j^x \sigma_{j+R}^x \rangle}{2} \quad (3.46)$$

where the inner spin-1 transverse string contributes with the sign prefactors. Thanks to hidden order in our reduced Hilbert space, the spin-1/2 configurations generated by σ^x represent the allowed spin-1 states and the forbidden ones are automatically filtered out. The coefficient 1/2 comes from the matrix elements of S^x at sites j and $j+R$.

3.4 Asymptotic decay laws

In the previous section we derived the expressions for the spin 1 string order parameters and correlation functions in terms of spin 1/2 operators. Now, thanks to the fact that the Hamiltonian (3.5) is quadratic in the fermionic operators, all the correlation functions can be evaluated using

Wick's theorem. Recalling some results from Section 1.1.2, we introduce [2] the operators $A_j = c_j^\dagger + c_j$ and $B_j = c_j^\dagger - c_j$ that allow to express the basic two-point correlations as

$$\langle \sigma_l^x \sigma_m^x \rangle = \langle B_l A_{l+1} B_{l+1} \cdots A_{m-1} B_{m-1} A_m \rangle$$

$$\langle \sigma_l^z \sigma_m^z \rangle = \langle A_l B_l A_m B_m \rangle$$

with $Q_{lm} \equiv \langle A_l A_m \rangle = \delta_{lm}$ and $S_{lm} = \langle B_l B_m \rangle = -\delta_{lm}$. If we further assume translational invariance (i.e. PBC) along the chain we have

$$\langle \sigma_l^x \sigma_m^x \rangle = \begin{vmatrix} G_{-1} & G_{-2} & \cdots & G_{l-m} \\ \vdots & & & \vdots \\ G_{m-l-2} & \cdots & & G_{-1} \end{vmatrix} \tag{3.47}$$

$$\langle \sigma_l^z \sigma_m^z \rangle = G_0^2 - G_{m-l} G_{l-m} \tag{3.48}$$

where $G_{-R} \equiv \langle B_j A_{j+R} \rangle = -\langle A_{j+R} B_j \rangle$. In particular, $G_0 = \langle (c_j^\dagger - c_j)(c_j^\dagger + c_j) \rangle = 2\langle n_j \rangle - 1 = \langle \sigma_j^z \rangle$, independent of j and $\langle \sigma_j^z \sigma_{j+R}^z \rangle = \langle \sigma_j^z \rangle^2 - G_R G_{-R}$. The R-dependence of $\mathcal{O}_z(R)$ and $\mathcal{O}_x(R)$ is given directly by $\langle \sigma_j^z \sigma_{j+R}^z \rangle$ and $\langle \sigma_j^x \sigma_{j+R}^x \rangle$ respectively. The ordinary correlators $\mathcal{C}_{x,z}(R)$ require a step more since they involve strings of Pauli operators. For example, each of the terms in equations (3.12) and (3.26) has the form $\langle \prod_k B_k A_k \rangle$. When $R \to \infty$ all the four terms in equation (3.12) tend to coincide so that

$$\mathcal{C}_z(R) \simeq (-1)^{R+1} G_H(R) = \langle B_j A_j B_{j+1} A_{j+1} \cdots B_{j+R-1} A_{j+R-1} B_{j+R} A_{j+R} \rangle.$$

Exploiting Wick's theorem, Caianiello and Fubini [6] have shown that the expectation value above can be expressed as a Pfaffian

$$\mathrm{Pf}\left|\begin{array}{cccccccccc} S_{-1} & S_{-2} & \cdots & S_{-R+1} & S_{-R} & G_0 & G_{-1} & \cdots & G_{-R+1} & G_{-R} \\ & S_{-1} & \cdots & S_{-R+2} & S_{-R+1} & G_1 & G_0 & \cdots & G_{-R+2} & G_{-R+1} \\ & & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ & & & S_{-1} & S_{-2} & G_{R-2} & G_{R-3} & \cdots & G_{-1} & G_{-2} \\ & & & & S_{-1} & G_{R-1} & G_{R-2} & \cdots & G_0 & G_{-1} \\ & & & & & G_R & G_{R-1} & \cdots & G_1 & G_0 \\ & & & & & & Q_{-1} & \cdots & Q_{-R+1} & Q_{-R} \\ & & & & & & & \ddots & \vdots & \vdots \\ & & & & & & & & Q_{-1} & Q_{-2} \\ & & & & & & & & & Q_{-1} \end{array}\right|$$

Thanks to the fact that $Q_{l\neq m} = S_{l\neq m} = 0$ this Pfaffian reduces to a Toeplitz determinant [15] and we get

$$\mathcal{C}_z(R) = \begin{vmatrix} -G_0 & -G_{-1} & \cdots & -G_{-R+1} & -G_{-R} \\ -G_1 & -G_0 & \cdots & -G_{-R+2} & -G_{-R+1} \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ -G_{R-1} & -G_{R-2} & \cdots & -G_0 & -G_{-1} \\ -G_R & -G_{R-1} & \cdots & -G_1 & -G_0 \end{vmatrix} \tag{3.49}$$

So, the determinants of the matrices with entries G_j becomes the central quantities of our analysis.

The matter is more complicated for the transverse spin-spin correlator. The fermionic version of equation (3.23) reads

$$\begin{aligned} \mathcal{C}_x &= \langle A_j \prod_{k<j} (1-2n_k) \prod_{k=j+1}^{j+R-1} (1-n_k) \prod_{k<j+R} (1-2n_k)\, A_{j+R}\rangle \\ &= \langle B_j \left(\prod_{k=j+1}^{j+R-1} c_k c_k^\dagger\right) A_{j+R}\rangle = \langle c_j^\dagger \left(\prod_{k=j+1}^{j+R-1} c_k c_k^\dagger\right) c_{j+R}^\dagger\rangle \end{aligned}$$

$$+\langle c_j^\dagger \left(\prod_{k=j+1}^{j+R-1} c_k c_k^\dagger\right) c_{j+R}\rangle - \langle c_j \left(\prod_{k=j+1}^{j+R-1} c_k c_k^\dagger\right) c_{j+R}^\dagger\rangle - \langle c_j \left(\prod_{k=j+1}^{j+R-1} c_k c_k^\dagger\right) c_{j+R}\rangle$$

After some algebra[2] we find that

$$\mathcal{C}_x = -\sqrt{\det \mathbf{M}_1} - \sqrt{\det \mathbf{M}_2} \tag{3.50}$$

where $\mathbf{M}_1$ and $\mathbf{M}_2$ are two block Toeplitz matrices defined in Appendix B. The calculation of the above correlator eventually involves a Toeplitz determinant generated by a matrix-valued symbol that may also become singular. As far as we know this case is not yet solved in the theory of Toeplitz determinants and in ref. [68] it has been suggested to extend directly the procedure valid in the nonsingular case. Fortunately in our case a workaround is possible: thanks to a suitable diagonalization, we are able to complete the calculation of the dominant contribution to $\mathcal{C}_x(R)$ in terms of a product of Toeplitz determinants, each one computed using the Fisher-Hartwig conjecture [18]. The details of this procedure are reported in Appendix B

[2] See Appendix B for details

3.4.1 Longitudinal string correlation $\mathcal{O}_z(R)$

The first object we will compute is the longitudinal string correlator. From equations (3.25) and (3.48) we get

$$\mathcal{O}_z(R) = -\frac{1}{4}\left[\left(1+\langle\sigma_j^z\rangle\right)^2 - G_R G_{-R}\right].$$

Following Barouch and McCoy [11] we express G_R as follows

$$G_R = -\frac{1}{2\pi}\int_0^{2\pi} dk \mathrm{e}^{-\mathrm{i}k(R+1)}\left[\frac{\left(1-\lambda_1^{-1}\mathrm{e}^{\mathrm{i}k}\right)\left(1-\lambda_2^{-1}\mathrm{e}^{\mathrm{i}k}\right)}{\left(1-\lambda_1^{-1}\mathrm{e}^{-\mathrm{i}k}\right)\left(1-\lambda_2^{-1}\mathrm{e}^{-\mathrm{i}k}\right)}\right]^{1/2} =$$

$$-\frac{1}{2\pi}\int_0^{2\pi} dk \mathrm{e}^{-\mathrm{i}kR} c(\mathrm{e}^{\mathrm{i}k}) \tag{3.51}$$

with

$$\lambda_{1,2} = \frac{h \pm \sqrt{h^2-(1-\gamma^2)}}{1-\gamma}. \tag{3.52}$$

and

$$c(\mathrm{e}^{\mathrm{i}k}) = \mathrm{e}^{-\mathrm{i}k}\sqrt{\frac{(1-\lambda_1^{-1}\mathrm{e}^{\mathrm{i}k})(1-\lambda_2^{-1}\mathrm{e}^{\mathrm{i}k})}{(1-\lambda_1^{-1}\mathrm{e}^{-\mathrm{i}k})(1-\lambda_2^{-1}\mathrm{e}^{-\mathrm{i}k})}}.$$

Note that since $\gamma > 1$ the two roots of the numerator are always real; the behaviour for $R \to \infty$ is controlled by λ_2. From equations (1.66), (1.69) and (1.68) we have, respectively:

- *Haldane phase* $h < 1 (\lambda_2 > 1)$

$$\mathcal{O}_z(R) \simeq \mathcal{O}_z + \frac{1}{8\pi}\frac{\mathrm{e}^{-2R/\xi}}{R^2}\ , \quad \xi \equiv 1/\ln\lambda_2$$

- *Critical line* $h = 1$ $(\lambda_2 = 1)$

$$\mathcal{O}_z(R) \simeq \mathcal{O}_z + \frac{1}{4\pi^2}\frac{1}{R^2}$$

- *Néel phase* $h > 1$ $(0 < \lambda_2 < 1)$

$$\mathcal{O}_z(R) \simeq \mathcal{O}_z + \frac{1}{8\pi}\frac{\mathrm{e}^{-2R/\xi}}{R^2}\ , \quad \xi \equiv -1/\ln\lambda_2$$

In every case the asymptotic value $\mathcal{O}_z \neq 0$ is simply interpreted as a non-saturated value of the magnetization along z in the XY model in transverse field

$$\mathcal{O}_z = -\frac{\left(1+\langle\sigma_j^z\rangle\right)^2}{4}, \tag{3.53}$$

where $\langle\sigma_j^z\rangle = G_0(h,\gamma)$ can be computed using equation (3.51) at $R = 0$.

3.4.2 Longitudinal spin-spin correlation function $\mathcal{C}_z(R)$ and pure string correlator $G_H(R)$

The asymptotic behaviour of the Toeplitz determinant in equation (3.49) can be found using the same technique as in [8], since (apart from a sign) the generating function of (3.49) is essentially the same used by Wu. Then we find:

- *Haldane phase* $h < 1$ ($\lambda_2 > 1$)

$$\mathcal{C}_z(R) \simeq (-1)^{R+1} G_H(R)$$

$$= \frac{1}{\sqrt{\pi}}(1-\lambda_1^{-2})^{1/4}(1-\lambda_2^{-2})^{-1/4}(1-\lambda_1^{-1}\lambda_2)^{-1/2}\frac{\mathrm{e}^{-R/\xi}}{R^{1/2}}$$

  which corresponds to the known decay behaviour at the isotropic Heisenberg point, as predicted by the nonlinear σ-model approach (see, for example, [69]). Moreover, in refs. [70, 71] it was argued that the same behaviour of the connected longitudinal correlation function persists also in presence of a staggered magnetic field; in this sense such a behaviour could be considered a signature of the Haldane phase, robust against anisotropic perturbations.

- *Critical line* $h = 1$ ($\lambda_2 = 1$)

$$\mathcal{C}_z(R) \simeq (-1)^{R+1} G_H(R) = \mathrm{e}^{1/4} 2^{1/12} \mathcal{A}^{-3} \frac{1}{(\gamma R)^{1/4}}$$

  where $\mathcal{A} = 1.282427130\ldots$ denotes Glaisher's constant [8].

- *Néel phase* $h > 1$ ($0 < \lambda_2 < 1$)

$$\mathcal{C}_z(R) \simeq (-1)^{R+1} G_H(R) = (1-\lambda_1^{-2})^{1/4}(1-\lambda_2^{2})^{1/4}(1-\lambda_1^{-1}\lambda_2)^{-1/2}$$

$$\cdot \left[1 + \frac{1}{2\pi(\lambda_2^{-1}-\lambda_2)^2}\frac{\mathrm{e}^{-2R/\xi}}{R^2}\right]$$

Apart from the nonzero asymptotic value for $h > 1$, that serves as an order parameter for the Nel phase (the ordered phase $T < T_\mathrm{c}$ in Wu's paper [8]), it must be noticed that both the power of R in the denominator and the exponential constant are different on the two sides of the transition. The roots $\lambda_{1,2}$ and the bulk correlation length ξ are the same as in subsec. 3.4.1 (see eq. (3.52)).

3.4.3 Transverse string correlation function $\mathcal{O}_x(R)$

- *Haldane phase* $h < 1$ ($\lambda_2 > 1$). The nonzero asymptotic value $\mathcal{O}_x$ comes from the long-range order $\lim_{R\to\infty}\langle\sigma_0^x\sigma_R^x\rangle$ in the XY model with spontaneous breaking of the symmetry $\sigma^x \to -\sigma^x$. The result can be borrowed directly from equation (4.1) of [11]

$$\mathcal{O}_x(R) \simeq -\frac{\left[\gamma^2(1-h^2)\right]^{1/4}}{1+\gamma}\left[1+\frac{1}{2\pi R^2}\frac{\mathrm{e}^{-2R/\xi}}{(\lambda_2-\lambda_2^{-1})^2}\right] \tag{3.54}$$

  with ξ having the same meaning of subsec. 3.4.1.

- *Critical line* $h = 1$ ($\lambda_2 = 1$). There is no long-range-order in $\langle\sigma_0^x\sigma_R^x\rangle$, that decays to zero as $R^{-1/4}$ as expected from the scaling dimension 1/8 of the primary operator in the $c = 1/2$ CFT [56]. Using equation (4.7) in [11] we have

$$\mathcal{O}_x(R) \simeq -\frac{\gamma}{1+\gamma}\mathrm{e}^{1/4}2^{1/12}\mathcal{A}^{-3}\frac{1}{(\gamma R)^{1/4}} \tag{3.55}$$

- *Néel phase* $h > 1$ ($0 < \lambda_2 < 1$). Equation (4.25) in ref. [11] is translated to

$$\mathcal{O}_x(R) \simeq -\frac{1}{2\sqrt{\pi}}\frac{\mathrm{e}^{-R/\xi}}{R^{1/2}}\left[(1-\lambda_2^2)^{-1}(1-\lambda_1^{-2})(1-\lambda_1^{-1}\lambda_2^{-1})^2\right]^{1/4}. \tag{3.56}$$

  We should stress that the critical exponent in equation (3.55) differs from the one in equations (3.54) and (3.56); it is not possible to recover the decay behaviour at $h = 1$ from the functions found for $h > 1$ or $h < 1$ simply by letting $R/\xi \to 0$ in the exponentials. Qualitatively, the reason is that the correlation functions should be described by a unique scaling function $\mathcal{F}(r)$ of the variable $r = R/\xi$, but the asymptotic expansions in the off-critical regime and in the critical regime are different. The former corresponds to $r \gg 1$ while the latter to $r \to 0$ for any large but finite value of R. A similar argument holds also for the longitudinal spin-spin correlation function $\mathcal{C}_z(R)$ of the previous subsection. Although possible in principle (see, for instance, [72] for the 2D classical Ising model), the derivation and the usage of the whole scaling functions is beyond the scope of this thesis. Finally, we notice from the equations above, as compared to those of subsec. (3.4.2), that the correlators $\mathcal{O}_x(R)$ and $\mathcal{C}_z(R)$ play a dual role above and below the transition line; when one order parameter is vanishing, the other is not. Here we do not have an explicitly duality relation between order and disorder lattice operators for the spin-1 model as in the Ising case (see, however, ref. [26] for the XY chain). Hence, what is a nontrivial fact is to see that also the decay laws interchange when the transition line is crossed.

3.4.4 Transverse spin-spin correlation $\mathcal{C}_x(R)$

The calculation of $\mathcal{C}_x$ is quite involved, so for the sake of brevity we will give only the results in this section, addressing the reader to Appendix B for the detailed calculation. From the analysis reported in Appendix B, we can prove a conjecture already put forth in ref. [59], namely that the transverse correlation function decays always exponentially even when one crosses the critical line. Here we can be more precise and derive also the power-law terms in front of the exponential

$$\mathcal{C}_x(R) \simeq \frac{\exp(-R/\Xi)}{R^{\eta_x}}\ , \quad \Xi \equiv \frac{2}{\beta+\beta'}, \tag{3.57}$$

where β and β' in the Haldane phase, along the critical line and in the Néel phase take, respectively, the form written in equations (B.5), (B.12), (B.8), (B.13), (B.9) and (B.15) in the Appendix. In particular we have checked that both β_c and β'_c for $h = 1$ and $\gamma \geq 1$ are nonzero. Hence, despite the fact that the system is critical, the transverse correlation function exhibits a *finite* characteristic length Ξ as it is also shown in Figure 3.2. As far as the exponent η_x is concerned:

- *Haldane phase* $h < 1$ $(\lambda_2 > 1)$ *and Néel phase* $h > 1$ $(\lambda_2 < 1)$: $\eta_x = 1/2$;

- *Critical line* $h = 1$ $(\lambda_2 = 1)$: $\eta_x = 1/4$. Despite the fact that $\Xi(h = 1) < \infty$, the algebraic prefactor is the same power-law that describes critical correlations in the quantum Ising model.

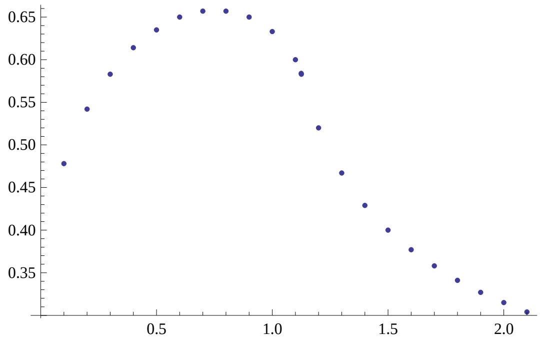

Figure 3.2: Behavior of the correlation lenght as a function of the anisotropy parameter λ: the points in the plot are found solving numerically the self-consistency equations (3.7), (3.8), (3.9) and plugging these results in (B.5), (B.12), (B.8), (B.13), (B.9) and (B.15).

From the values of h and γ reported in the last two columns of table 3.2 we have computed $\Xi[h(\lambda, D), \gamma(\lambda, D)]$; for example when $\lambda = 1$ we find that Ξ decreases steadily as D is decreased towards larger negative values, passing from the Haldane to the Néel phase. This behaviour is consistent with the numerical best-fit estimates of Ξ made in the section 3.6.

3.5 λ-D model with a biquadratic interaction

We now generalize the λ-D model (3.2) studied so far, including a biquadratic term

$$\mathcal{H}_{AKLT} = \mathcal{H}_{\lambda-D} - \sum_{j=1}^{N} \left[\beta \left(\mathbf{S_j} \cdot \mathbf{S_{j+1}}\right)^2\right] \tag{3.58}$$

where $\mathcal{H}_{\lambda-D}$ is the hamiltonian (3.2). We notice that setting $\lambda = 1$, $D = 0$ the hamiltonian (3.58) reduces to the general bilinear biquadratic Heisenberg hamiltonian. As already mentioned in Chapter 2 this hamiltonian is exactly the hamiltonian of the AKLT model [42] at $\beta = -1/3$ and it is known to be solvable at $\beta = 1$ [36], [37] and at $\beta = -1$ [73], [74]. Assuming hidden antiferromagnetic order we will map (3.58) onto spinless fermions. Let's consider in detail the biquadratic term

$$(\mathbf{S_j}\cdot\mathbf{S_{j+1}})^2 = \left[\frac{1}{2}\left(S_j^+S_{j+1}^- + S_j^-S_{j+1}^+\right) + S_j^zS_{j+1}^z\right]^2 =$$

$$\frac{1}{4}\left(S_j^+S_{j+1}^- + S_j^-S_{j+1}^+\right)^2 + \left(S_j^zS_{j+1}^z\right)^2 +$$

$$\frac{1}{2}\left(S_j^+S_{j+1}^- + S_j^-S_{j+1}^+\right)S_j^zS_{j+1}^z + \frac{1}{2}S_j^zS_{j+1}^z\left(S_j^+S_{j+1}^- + S_j^-S_{j+1}^+\right) =$$

$$\frac{1}{4}\left[\left(S_j^+S_{j+1}^-\right)^2 + \left(S_j^-S_{j+1}^+\right)^2 + S_j^+S_{j+1}^-S_j^-S_{j+1}^+ + S_j^-S_{j+1}^+S_j^+S_{j+1}^-\right] + \left(S_j^zS_{j+1}^z\right)^2$$

$$+\frac{1}{2}\left(S_j^+S_{j+1}^- + S_j^-S_{j+1}^+\right)S_j^zS_{j+1}^z + \frac{1}{2}S_j^zS_{j+1}^z\left(S_j^+S_{j+1}^- + S_j^-S_{j+1}^+\right) \quad (3.59)$$

Let's study now each term of (3.59)

- $\left(S_j^+S_{j+1}^-\right)^2 = 0$ since it does not preserve string order. Its action is in fact given by

$$j=\uparrow \quad j+1 = \left[\begin{array}{ccc} 0 & \rightarrow & \emptyset \\ \downarrow & \rightarrow & \emptyset \end{array}\right.$$

$$j=0 \quad j+1 = \left[\begin{array}{ccc} \uparrow & \rightarrow & \emptyset \\ 0 & \rightarrow & \emptyset \\ \downarrow & \rightarrow & \emptyset \end{array}\right.$$

$$j=\downarrow \quad j+1 = \left[\begin{array}{ccc} \uparrow & \rightarrow & \uparrow_j\downarrow_{j+1} \\ 0 & \rightarrow & \emptyset \end{array}\right.$$

- Similarly $\left(S_j^-S_{j+1}^+\right)^2 = 0$.
- We shall now verify that

$$\mathcal{D} = \frac{1}{4}\left(S_j^+S_{j+1}^-S_j^-S_{j+1}^+ + S_j^-S_{j+1}^+S_j^+S_{j+1}^-\right)$$

$$= \mathcal{P}_{++} + \mathcal{P}_{+-} + \mathcal{P}_{-+} + 2\mathcal{P}_{--} = 2 - n_j - n_{j+1} + n_jn_{j+1}$$

where we have defined

$$\mathcal{P}_{++} = n_j n_{j+1} \qquad \mathcal{P}_{+-} = n_j \left(1 - n_{j+1}\right)$$

$$\mathcal{P}_{-+} = \left(1 - n_j\right) n_{j+1} \qquad \mathcal{P}_{--} = \left(1 - n_j\right)\left(1 - n_{j+1}\right) \tag{3.60}$$

The action of $\mathcal{D}$ on configuration with string order is in fact given by

$$j = \uparrow \quad j+1 = \left[\begin{array}{ccc} 0 & \rightarrow & \uparrow_j 0_{j+1} \\ \downarrow & \rightarrow & \uparrow_j \downarrow_{j+1} \end{array}\right.$$

$$j = 0 \quad j+1 = \left[\begin{array}{ccc} \uparrow & \rightarrow & 0_j \uparrow_{j+1} \\ 0 & \rightarrow & 2\left(0_j 0_{j+1}\right) \\ \downarrow & \rightarrow & 0_j \downarrow_{j+1} \end{array}\right.$$

$$j = \downarrow \quad j+1 = \left[\begin{array}{ccc} \uparrow & \rightarrow & \downarrow_j \uparrow_{j+1} \\ 0 & \rightarrow & \downarrow_j 0_{j+1} \end{array}\right.$$

- It is straightforward that $\left(S_j^z S_{j+1}^z\right)^2 = n_j n_{j+1}$
- Finally, we see that

$$\frac{1}{2}\left[S_j^z S_{j+1}^z \left(S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+\right)\right] = -c_j^\dagger c_{j+1}^\dagger$$

since its action is given by

$$j = \uparrow \quad j+1 = \left[\begin{array}{ccc} 0 & \rightarrow & \emptyset \\ \downarrow & \rightarrow & \emptyset \end{array}\right.$$

$$j = 0 \quad j+1 = \left[\begin{array}{ccc} \uparrow & \rightarrow & \emptyset \\ 0 & \rightarrow & -\uparrow_j \downarrow_j - \downarrow_j \uparrow_{j+1} \\ \downarrow & \rightarrow & \emptyset \end{array}\right.$$

$$j = \downarrow \quad j+1 = \left[\begin{array}{ccc} \uparrow & \rightarrow & \emptyset \\ 0 & \rightarrow & \emptyset \end{array}\right.$$

- and its hermitean conjugate $\left(S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+\right) S_j^z S_{j+1}^z = -2c_{j+1}c_j$

Collecting all terms the hamiltonian (3.58) becomes

$$\mathcal{H}_f = \sum_{j=1}^{N} \left[\left(c_j^\dagger c_{j+1} + (1+\beta)\, c_j^\dagger c_{j+1}^\dagger + h.c. \right) + \right.$$

$$\left. - (\lambda + 2\beta)\, n_j n_{j+1} + (D + 2\beta)\, n_j - 2\beta \right] \tag{3.61}$$

that is, apart from a constant term and a redefinition of the constant prefactors, exactly the same as (3.4). Following the same steps as in (3.2) we get the effective hamiltonian

$$\mathcal{H}_{hf} = \sum_i \left[\left(c_i^\dagger c_{i+1} + \gamma c_i^\dagger c_{i+1}^\dagger + h.c. \right) - h c_i^\dagger c_i \right] + const. \tag{3.62}$$

with the anisotropy constant γ and the magnetic field defined by

$$h \equiv \frac{2\,(\lambda + 2\beta)\, n_0 - (D + 2\beta)}{2\,(1 + (\lambda + 2\beta)\, A)} \qquad \gamma \equiv \frac{1 - (\lambda + 2\beta)\, B + \beta}{1 + (\lambda + 2\beta)\, A} \tag{3.63}$$

where n_0, A and B are again solutions of the self-consistency equations (3.7), (3.8), (3.9).At $\lambda = 1$, $D = 0$ and $\beta = -1/3$ these equations are solved self-consistently by the analytical solution $n_0 = 2/3$, $A = B = -2/9$; we obtain $h = 3/5$ e $\gamma = 4/5$ and thus $\lambda_1 = \lambda_2$ (with λ_1, λ_2 defined as in (3.52)). With the above data, we get that the longitudinal string order parameter

$$\mathcal{O}_z = -\frac{1}{4}\left(1 + \langle \sigma^z \rangle\right)^2$$

where

$$\langle \sigma^z \rangle = G_0 = -\frac{1}{2\pi} \int_0^{2\pi} dk e^{-ik} \sqrt{\frac{\left(1 - \lambda_1^{-1} e^{ik}\right)\left(1 - \lambda_2^{-1} e^{ik}\right)}{\left(1 - \lambda_1^{-1} e^{-ik}\right)\left(1 - \lambda_2^{-1} e^{-ik}\right)}}$$

is $\mathcal{O}_z = 4/9$ that is exactly the same value found analitycally for the AKLT model [43]. Interestingly enough even if the XY model does not have an explicit rotational symmetry as the original spin 1 hamiltonian, we find again $\mathcal{O}_x = -4/9$. This accordance can be taken as a positive check of our approach.

3.6 Comparison with DMRG results

The results of the previous section regarding the long-distance decay of ordinary and string correlation functions are summarized in table 3.3 where:

$$f_0(R) = A_0 \frac{\exp(-R/A_1)}{R^{1/4}} \tag{3.64}$$

$$f_1(R) = A_2 + A_0 \frac{\exp(-R/A_1)}{\sqrt{R}} \tag{3.65}$$

$$f_2(R) = A_2 + A_0 \frac{\exp(-2R/A_1)}{R^2}. \tag{3.66}$$

Within the approximation of hidden order and for large R these asymptotic laws are to be considered exact and valid for the Haldane and Néel phases and associated transition line as specified in table 3.3. It should be noted that $f_1(R)$ and $f_2(R)$ agree with the general form argued for the d-dimensional Ising model (see, for example, [75] and refs. therein) although the derivation of the latter did not include the case of string correlation functions.

The two functional forms $f_{1,2}$ now can be used to extract, for example, the asymptotic value of string order correlation functions computed numerically; in this sense A_0, A_1 and A_2 may be regarded as free fitting parameters. The goodness of the best-fit procedure can be assessed by computing the reduced χ^2:

$$\tilde{\chi}^2 \equiv \frac{\sum \text{squares of differences}}{\#\text{ of data points} - \#\text{ of fit parameters} - 1}.$$

Clearly one could use many other different functions to extrapolate the correlators to $R \to \infty$. However, as recalled in the introduction, the literature contains very few, empirical, information about the asymptotic approach to the limit values of the string correlation functions. Our study was motivated by this fact and so here we perform a comparison between f_0, f_1 and f_2 by examining their capability to fit the spin-spin and string correlations evaluated numerically through the DMRG. Actually, following the idea of ref. [69], in order to take into account the PBC we employ the left-right symmetrized expressions of equations (3.64)-(3.66)

$$F_\ell(R) \equiv \frac{f_\ell(R) + f_\ell(L-R)}{2}, \ \ell = 0, 1, 2, \tag{3.67}$$

Phase	C.f.	Decay law
Haldane	$\mathcal{C}_z$	$f_1(A_2 \equiv 0)$
Transition	$\mathcal{C}_z$	f_0 $(A_1^{-1} = 0)$
Néel	$\mathcal{C}_z$	f_2
Haldane	$\mathcal{C}_x$	$f_1(A_2 \equiv 0)$
Transition	$\mathcal{C}_x$	f_0
Néel	$\mathcal{C}_x$	$f_1(A_2 \equiv 0)$
Haldane	$\mathcal{O}_z$	f_2
Transition	$\mathcal{O}_z$	f_2 $(A_1^{-1} = 0)$
Néel	$\mathcal{O}_z$	f_2
Haldane	$\mathcal{O}_x$	f_2
Transition	$\mathcal{O}_x$	f_0 $(A_1^{-1} = 0)$
Néel	$\mathcal{O}_x$	$f_1(A_2 \equiv 0)$

Table 3.3: Expected asymptotic behaviour of string ($\mathcal{O}$) and usual ($\mathcal{C}$) correlation functions in the Haldane and Néel phases of model (3.2) and along the critical transition line separating them. The fitting functions $f_{0,1,2}$ are defined in equations (3.64)-(3.66). Note the interchanged role of $\mathcal{O}_x(R)$ and $\mathcal{C}_z(R)$ above and below the transition line.

at least for the correlation functions in the z-channel. As regards $\mathcal{O}_x$, while translational invariance implies that it depends on the difference between the sites at the ends of the string, it is not always guaranteed that it depends only on the distance on the ring. In other terms the expectation value

$$\langle S_i^x \mathrm{e}^{\mathrm{i}\pi \sum_{k=i+1}^{j-1} S_k^x} S_j^x \rangle$$

may differ from the same expression with i and j interchanged. In fact, using the properties of the exponentials of spin-1 operators, $\exp(\mathrm{i}\pi S_i^x) = \exp(-\mathrm{i}\pi S_i^x)$ and $S_i^x \exp(\mathrm{i}\pi S_i^x) = -S_i^x$, it can be shown that the expression above can rewritten as

$$\langle S_j^x \mathrm{e}^{\mathrm{i}\pi \sum_{k=j+1}^{i-1} S_k^x} S_i^x \mathrm{e}^{\mathrm{i}\pi S_{\mathrm{tot}}^x} \rangle$$

where $S_{\mathrm{tot}}^x = \sum_{i=1}^{L} S_i^x$. The point is that in general the GS of an anisotropic spin chain is not invariant under the action of $\exp(\mathrm{i}\pi S_{\mathrm{tot}}^x)$ and so a direct inspection is required case by case in order to decide if a symmetrized fitting function has to be used or not.

The asymptotic limits (i.e. the values of A_2) resulting from of a series of best-fits made on DMRG data obtained by fixing $\lambda = 1$ and letting D to vary across the Haldane-Néel transition from -0.125 to -0.875 are plotted in figure 3.3. It is seen that the nonvanishing values of $\mathcal{O}_x$ and M_z characterize, respectively, the Haldane and the Néel phase. It is reasonable to expect that the location of the critical point as the value of D at which the two order parameters vanish leads to two slightly different estimates. However, with more accurate methods the critical point was previously found to be $D_{\mathrm{c}} = -0.315$ [54, 61].

In the simulations we have fixed the total length of the chain to be $L = 100$ sites and computed the GS properties by retaining from 243 to 324 DMRG states in the sector with $S_{\mathrm{tot}}^z = 0$, which is the only good quantum number that we could use. All the functional forms derived above are asymptotic so we cannot expect them to be reliable for very short distances. Therefore, we have conventionally excluded the data with $R \leq 5$ from the fitted points. In the Néel phase the GS tends to become doubly degenerate in the limit $L \to \infty$; in order to take into account this difficulty we have built the reduced density matrix by targeting the two low-lying states rather

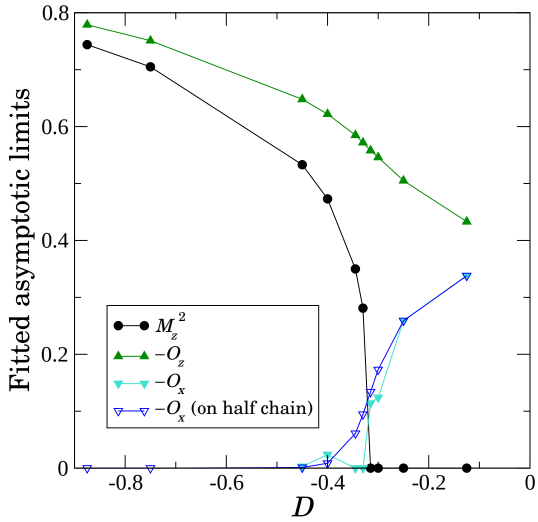

Figure 3.3: Asymptotic values (order parameters) attained by $\mathcal{C}_z$ (dots), $\mathcal{O}_z$ (up triangles) and $\mathcal{O}_x$ (down triangles). The limits to $R \to \infty$ correspond to the values of the best-fit parameters A_2 for the fitting function that, case by case, gives the smallest value of $\tilde{\chi}^2$. The empty triangles result from fitting the transverse string correlation functions on half chain (see text for explanation).

than just the GS. Finally we have performed three finite-system sweeps to achieve a better accuracy. In the cases we have considered, the transverse string correlation $\mathcal{O}_x(R)$ turned out to be symmetric with respect to the middle of the chain except for $D = -0.75$ and $D = -0.875$. For this reason we have repeated the fit using directly the functions of equations (3.64), (3.65) and (3.66) without symmetrization selecting only the points in the first half of the chain. The asymptotic values are essentially unaffected, with the exception of those referring to the critical point. In general when the results of the fit are such that $A_1 \gg L$ (typically close to criticality) we conclude that the exponential tail of the fitting function is essentially saturated to unity and an algebraic fit would produce the same result.

As far as the best-fitting functions for $\mathcal{C}_z(R)$ and $\mathcal{O}_x(R)$ are concerned, the passage from the type f_1 to the type f_2 going through f_0 at the critical point, as in table 3.3, actually takes place gradually in the interval $D \in (-0.345, -0.315)$, the worst values of $\tilde{\chi}^2$ being of order 10^{-5}. The best choice to fit the transverse spin-spin correlation function $\mathcal{C}_x(R)$, instead, follows the prediction of table 3.3 (F_1 except at the critical line, where it becomes F_0) with a deviation $\tilde{\chi}^2 < 10^{-8}$. Finally, the longitudinal string correlator $\mathcal{O}_z(R)$ is very well fitted by F_2, in agreement with table 3.3, with $\tilde{\chi}^2 \sim 10^{-9}$ or better.

It is also important to check quantitatively the goodness of the Hartree-Fock approximation. The decoupling parameter in the fermionic version are $n_0 = \langle n_{j=0}\rangle$, $A = \langle c_1^\dagger c_0\rangle$ and $B = \langle c_1 c_0\rangle$ where we have selected a reference site "0" invoking translational invariance. In the original spin-1 formalism it can be checked directly that

$$n_0 = \langle (S_0^z)^2\rangle \ , \ \ A = \frac{1}{2}\langle S_1^z \left(S_0^+ S_1^- + S_1^+ S_0^-\right) S_0^z\rangle \tag{3.68}$$

The operator $c_1 c_0$ destroys a couple of fermions in adjacent sites; in the spin language they could be $\uparrow\downarrow$ or $\downarrow\uparrow$ depending on the surrounding sites in order to respect the AFM order. Let us express the GS in the form $|\mathrm{GS}\rangle = \alpha|\Uparrow\rangle + \beta|\Downarrow\rangle$, where $|\Uparrow\rangle$ denotes a linear combination of states in which the first nonzero spin along-z is directed upward and $|\Downarrow\rangle$ the same state with all the spin reversed. Only one of the terms in $\left(S_0^+ S_1^- + S_1^+ S_0^-\right)$ will act on $|\Uparrow\rangle$ respecting the AFM order and the other term will thereby

λ	D	$n_{0,\mathrm{DMRG}}$	A_{DMRG}	B_{DMRG}	$n_{0,\mathrm{s-c}}$	$A_{\mathrm{s-c}}$	$B_{\mathrm{s-c}}$
1	0	0.667	−0.166	−0.30080	0.709	−0.158	−0.253
1	−0.125	0.702	−0.151	−0.28908	0.745	−0.137	−0.246
1	−10	0.996	−0.000324	−0.0442	0.996	−0.000317	−0.0433
5	−0.125	0.991	−0.000860	−0.0654	0.991	−0.000853	−0.0649

Table 3.4: DMRG ($L = 100$) versus self-consistent (s-c) estimates of the three decoupling parameters n_0, A and B of equations (3.68) and (3.69). It must be kept in mind that the continuum versions of the self-consistent equations neglect some $O(L^{-1})$ terms coming from isolated contributions at wavenumber 0 or π.

act on $|\Downarrow\rangle$. When the scalar product with $\langle\mathrm{GS}|$ is taken, the states from $|\Uparrow\rangle$ will not mix with those from $|\Downarrow\rangle$. Therefore we try with the expression

$$B = -\frac{1}{2}\langle\left(S_0^- S_1^+ + S_0^+ S_1^-\right) S_0^z S_1^z\rangle. \tag{3.69}$$

In table 3.4 we report the values of the decoupling parameters for a set of points in the Haldane and Néel phases, comparing the DMRG values with the numerical solution of the self-consistent equations using 100 iterations from different choices of initial conditions. Having the DMRG estimates for n_0 and A we may also produce a “hybrid” estimate of the critical point by setting $h = 1$ in equation (3.6) and then solving for $\tilde{D}_\mathrm{c}(\lambda) = 2[\lambda(n_{0,\mathrm{DMRG}} - A_{\mathrm{DMRG}}) - 1]$. With $\lambda = 1$ we find for example $\tilde{D}_\mathrm{c} = -0.254$, that compares slightly better than the fully-self-consistent value ($D_\mathrm{c} = -0.214$) to the accepted numerical one $D_\mathrm{c} \cong -0.315$.

Apart from the value n_0, which quantifies the number of spins with nonzero projection along z, we expect that the goodness of the mapping used in this work is higher when the hidden order is larger.

Chapter 4

Entanglement in the λ-D model

Entanglement [77], [78] is one of the most intriguing features of composite quantum systems connected to the tensor product structure of the underlying Hilbert space of states. A mixed state of a bipartite quantum system described by some density matrix ρ is said to be entangled or inseparable if ρ cannot be written as a convex linear combination of product states, otherwise it is called classically correlated or separable.

The characterization and quantification of entanglement in mixed quantum states is a highly non trivial problem. It is even difficult to formulate simple operational criteria which allow a unique identification of all separable states of a given composite system. There exist however many separability criteria: a simple and very strong criterion is the Peres-Horodecki criterion [79], [80], which states that a necessary and sufficient condition for a mixed state of a bipartite system to be separable is that its partial transpose with respect to one of the subsystems is positive. This criterion is necessary and sufficient if the Hilbert space of the bipartite system has dimension 2×2 and 2×3. In general, for larger dimension, this condition is just necessary but not sufficient. In principle it is possible to have inseparable states having a positive partial transpose, the so called *bound entangled* states [81], [82].

The analysis of the entanglement structure is greatly simplified through the introduction of symmetries, i.e. if we restrict ourselves to those states of the composite system which are invariant under certain groups of symmetry transformations. It can be shown [83], [84], [85], [86], [87] then that the Peres-Horodecki criterion is necessary and sufficient for $SU(2)$-invariant states on a bipartite Hilbert space with dimensions $2 \times N$, $3 \times M$ (M being odd) and 4×4 respectively.

Vidal and Werner [89] introduced a computable measure of entanglement based on the trace norm of the partial transpose ρ^{T_A} of the bipartite mixed state ρ. It measures the degree to which ρ^{T_A} fails to be positive, and it can be regarded as a quantitative version of the Peres-Horodecki criterion. They introduced the negativity[1] [89]

$$\mathcal{N}(\rho) \equiv \frac{\left\|\rho^{T_A}\right\|_1 - 1}{2} = \sum_i |\mu_i| \tag{4.1}$$

which corresponds to the absolute value of the sum of negative eigenvalues of ρ^{T_A} (μ_i being a negative eigenvalue of ρ^{T_A}), and which vanishes for unentangled states. They furthermore proved [89] that $\mathcal{N}(\rho)$ is an entanglement monotone, and as such it can be used to quantify the degree of entanglement in composite systems.

In this chapter we will first compute an analytical expression for the negativity of the λ-D model obtaining a result in agreement with reference [88]; then, using the mapping between spin 1 and spinless fermions introduced in the previous chapter, we are able to express the negativity of the model in terms of fermionic correlators. In particular, we find that all the eigenvalues of the partial transpose ρ^T can be expressed in terms of the spin-spin and string correlators already calculated in the previous chapter. We find that the negativity of the λ-D model goes asymptotically to 0, i.e. as the distance between the two subsystems becomes large.

4.1 Two site density matrix of the λ-D model

We consider the spin 1 XXZ model with an on site anisotropy

$$\mathcal{H} = \sum_{j=1}^{N} \left[S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \lambda S_j^z S_{j+1}^z + D \left(S_j^z\right)^2 \right] \tag{4.2}$$

[1] $\|\cdot\|_1$ denotes the trace norm

Let's consider the two site density matrix; we shall use a basis of eigenstates of S^z ordered as $|\uparrow\rangle|\uparrow\rangle$, $|\uparrow\rangle|0\rangle$, $|0\rangle|\uparrow\rangle$, $|\uparrow\rangle|\downarrow\rangle$, $|0\rangle|0\rangle$, $|\downarrow\rangle|\uparrow\rangle$, $|0\rangle|\downarrow\rangle$, $|\downarrow\rangle|0\rangle$, $|\downarrow\rangle|\downarrow\rangle$. In this basis the density matrix is block diagonal

$$\rho = \begin{pmatrix} A_{11} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & A_{22} & A_{23} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & A_{32} & A_{33} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & A_{44} & A_{45} & A_{46} & 0 & 0 & 0 \\ 0 & 0 & 0 & A_{54} & A_{55} & A_{56} & 0 & 0 & 0 \\ 0 & 0 & 0 & A_{64} & A_{65} & A_{66} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & A_{77} & A_{78} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & A_{87} & A_{88} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & A_{99} \end{pmatrix}$$

It is straightforward to verify that the following are symmetries of the hamiltonian

$$\mathcal{R}_z(\alpha) = e^{i\alpha\sum_k S_k^z} \qquad \mathcal{R}_{x,y}(\pi) = e^{i\pi\sum_k S_k^{x,y}} \tag{4.3}$$

We have the 0 entries since, for example

$$A_{12} = \mathrm{tr}\left(|\uparrow\rangle\langle\uparrow|_i \otimes |0\rangle\langle\uparrow|_j \rho\right)$$

$$= \mathrm{tr}\left(\mathcal{R}_z^{-1}(\alpha)\,|\uparrow\rangle\langle\uparrow|_i \otimes |0\rangle\langle\uparrow|_j \mathcal{R}_z(\alpha)\,\rho\right) = e^{-i\alpha}A_{12}$$

since $\mathcal{R}_z(\alpha)$ is a symmetry $\forall\alpha$ it must be $A_{12} = 0$.

The two site density matrix can be further symplified; taking into account invariance under the exchange $i \leftrightarrow j$ we have

$$A_{22} = \mathrm{tr}\left(|\uparrow\rangle\langle\uparrow|_i \otimes |0\rangle\langle 0|_j \rho\right) = \mathrm{tr}\left(|0\rangle\langle 0|_i \otimes |\uparrow\rangle\langle\uparrow|_j \rho\right) = A_{33} \tag{4.4}$$

$$A_{32} = \mathrm{tr}\left(|\uparrow\rangle\langle 0|_i \otimes |0\rangle\langle\uparrow|_j \rho\right) = \mathrm{tr}\left(|0\rangle\langle\uparrow|_i \otimes |\uparrow\rangle\langle 0|_j \rho\right) = A_{32}^{\dagger} = A_{23} \tag{4.5}$$

$$A_{44} = \mathrm{tr}\left(|\uparrow\rangle\langle\uparrow|_i \otimes |\downarrow\rangle\langle\downarrow|_j \rho\right) = \mathrm{tr}\left(|\downarrow\rangle\langle\downarrow|_i \otimes |\uparrow\rangle\langle\uparrow|_j \rho\right) = A_{66} \tag{4.6}$$

$$A_{54} = \mathrm{tr}\left(|\uparrow\rangle\langle 0|_i \otimes |\downarrow\rangle\langle 0|_j \rho\right) = \mathrm{tr}\left(|\downarrow\rangle\langle 0|_i \otimes |\uparrow\rangle\langle 0|_j \rho\right) = A_{56} \tag{4.7}$$

$$A_{64} = \mathrm{tr}\left(| \uparrow\rangle\langle\downarrow |_i \otimes | \downarrow\rangle\langle\uparrow |_j \rho\right) = \mathrm{tr}\left(| \downarrow\rangle\langle\uparrow |_i \otimes | \uparrow\rangle\langle\downarrow |_j \rho\right) = A_{46} \tag{4.8}$$

$$A_{45} = \mathrm{tr}\left(|0\rangle\langle\uparrow |_i \otimes |0\rangle\langle\downarrow |_j \rho\right) = \mathrm{tr}\left(|0\rangle\langle\downarrow |_i \otimes |0\rangle\langle\uparrow |_j \rho\right) = A_{54}^{\dagger} = A_{65} \tag{4.9}$$

$$A_{77} = \mathrm{tr}\left(|0\rangle\langle 0|_i \otimes | \downarrow\rangle\langle\downarrow |_j \rho\right) = \mathrm{tr}\left(| \downarrow\rangle\langle\downarrow |_i \otimes |0\rangle\langle 0|_j \rho\right) = A_{88} \tag{4.10}$$

$$A_{87} = \mathrm{tr}\left(|0\rangle\langle\downarrow |_i \otimes | \downarrow\rangle\langle 0|_j \rho\right) = \mathrm{tr}\left(| \downarrow\rangle\langle 0|_i \otimes |0\rangle\langle\downarrow |_j \rho\right) = A_{87}^{\dagger} = A_{78} \tag{4.11}$$

Next we use the symmetry $\mathcal{R}_x(\pi)$

$$A_{11} = \mathrm{tr}\left(\mathcal{R}_x^{-1}(\pi) | \uparrow\rangle\langle\uparrow |_i \otimes | \uparrow\rangle\langle\uparrow |_j \mathcal{R}_x(\pi)\,\rho\right)$$

$$= \mathrm{tr}\left(| \downarrow\rangle\langle\downarrow |_i \otimes | \downarrow\rangle\langle\downarrow |_j \rho\right) = A_{99} \tag{4.12}$$

$$A_{22} = \mathrm{tr}\left(\mathcal{R}_x^{-1}(\pi) | \uparrow\rangle\langle\uparrow |_i \otimes |0\rangle\langle 0|_j \mathcal{R}_x(\pi)\,\rho\right)$$

$$= \mathrm{tr}\left(| \downarrow\rangle\langle\downarrow |_i \otimes |0\rangle\langle 0|_j \rho\right) = A_{77} \tag{4.13}$$

$$A_{23} = \mathrm{tr}\left(\mathcal{R}_x^{-1}(\pi) | \uparrow\rangle\langle 0|_i \otimes |0\rangle\langle\uparrow |_j \mathcal{R}_x(\pi)\,\rho\right)$$

$$= \mathrm{tr}\left(| \downarrow\rangle\langle 0|_i \otimes |0\rangle\langle\downarrow |_j \rho\right) = A_{78} \tag{4.14}$$

The density matrix takes then the form

$$\rho = \begin{pmatrix} A_{11} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & A_{22} & A_{23} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & A_{23} & A_{22} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & A_{44} & A_{45} & A_{46} & 0 & 0 & 0 \\ 0 & 0 & 0 & A_{45}^{\dagger} & A_{55} & A_{45}^{\dagger} & 0 & 0 & 0 \\ 0 & 0 & 0 & A_{46} & A_{45} & A_{44} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & A_{22} & A_{23} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & A_{23} & A_{22} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & A_{11} \end{pmatrix} \tag{4.15}$$

Noticing that

$$|0\rangle\langle 0| = 1 - (S^z)^2$$

$$|\uparrow\rangle\langle\uparrow| = \frac{(S^z)^2 + S^z}{2} \qquad |\downarrow\rangle\langle\downarrow| = \frac{(S^z)^2 - S^z}{2}$$

$$|\uparrow\rangle\langle 0| = \frac{S^z S^+}{\sqrt{2}} \qquad |\downarrow\rangle\langle 0| = \frac{S^z S^-}{\sqrt{2}}$$

we can now explicitely write down the matrix entries in term of spin operators[2]

$$A_{11} = \frac{1}{4}\langle\left[(S^z)^2 + S^z\right]_i \otimes \left[(S^z)^2 + S^z\right]_j\rangle = \frac{1}{4}\left[\langle(S_i^z)^2 \otimes \left(S_j^z\right)^2\rangle + \langle S_i^z \otimes S_j^z\rangle\right] \tag{4.16}$$

$$A_{22} = \frac{1}{2}\langle\left[(S^z)^2 + S^z\right]_i \otimes \left[(1 - S^z)^2\right]_j\rangle = \frac{1}{2}\left[\langle(S_i^z)^2 \otimes 1\rangle - \langle(S_i^z)^2 \otimes \left(S_j^z\right)^2\rangle\right] \tag{4.17}$$

$$A_{23} = \frac{1}{4}\langle S_i^z S_i^+ \otimes S_j^- S_j^z + S_i^- S_i^z \otimes S_j^z S_j^+\rangle \tag{4.18}$$

$$A_{44} = \frac{1}{4}\langle\left[(S^z)^2 + S^z\right]_i \otimes \left[(S^z)^2 - S^z\right]_j\rangle = \frac{1}{4}\left[\langle(S_i^z)^2 \otimes \left(S_j^z\right)^2\rangle - \langle S_i^z \otimes S_j^z\rangle\right] \tag{4.19}$$

$$A_{45} = -\frac{1}{2}\langle S_i^z S_i^+ \otimes S_j^z S_j^-\rangle \tag{4.20}$$

$$A_{46} = \frac{1}{8}\langle(S_i^+)^2 \otimes \left(S_j^-\right)^2 + (S_i^-)^2 \otimes \left(S_j^+\right)^2\rangle \tag{4.21}$$

$$A_{55} = \langle\left[1 - (S^z)^2\right]_i \otimes \left[1 - (S^z)^2\right]_j\rangle \tag{4.22}$$

The partial transpose of (4.15) with respect to the second subsystem is

$$\rho^{T_2} = \begin{pmatrix} A_{11} & 0 & 0 & 0 & A_{23} & 0 & 0 & 0 & A_{46} \\ 0 & A_{22} & 0 & 0 & 0 & 0 & A_{45} & 0 & 0 \\ 0 & 0 & A_{22} & 0 & 0 & 0 & 0 & A_{45}^\dagger & 0 \\ 0 & 0 & 0 & A_{44} & 0 & 0 & 0 & 0 & 0 \\ A_{23} & 0 & 0 & 0 & A_{55} & 0 & 0 & 0 & A_{23} \\ 0 & 0 & 0 & 0 & 0 & A_{44} & 0 & 0 & 0 \\ 0 & A_{45}^\dagger & 0 & 0 & 0 & 0 & A_{22} & 0 & 0 \\ 0 & 0 & A_{45} & 0 & 0 & 0 & 0 & A_{22} & 0 \\ A_{46} & 0 & 0 & 0 & A_{23} & 0 & 0 & 0 & A_{11} \end{pmatrix}$$

[2]It can be checked immediately that $(S_i^z)^2 \otimes S_j^z = S_i^z \otimes \left(S_j^z\right)^2 = 0$

and its eigenvalues are given by

$$\lambda_1 = \lambda_2 = A_{44}$$

$$\lambda_{3,4} = \lambda_{5,6} = \left[A_{22} \pm \sqrt{A_{45}A_{45}^\dagger}\right]$$

$$\lambda_{7,8} = \frac{1}{2}\left[A_{11} + A_{46} + A_{55} \pm \sqrt{(A_{11} + A_{46} - A_{55})^2 + 8A_{23}^2}\right]$$

$$\lambda_9 = A_{11} - A_{46}$$

4.2 Mapping for the density matrix elements

Now we will map the above spin 1 quantities in terms of spin 1/2 expectation values, using the effective mapping between spin 1 chains and integrable fermions discussed in Chapter 3. Let's consider a state

$$|\Psi\rangle = |\psi_1\rangle + \psi_2\rangle$$

where

$$|\psi_1\rangle = |\cdots 0 \uparrow 0 \cdots 0 \downarrow 0 \cdots 0 \uparrow 0 \cdots 0 \downarrow 0 \cdots 0 \uparrow 0 \cdots\rangle$$

$$|\psi_2\rangle = |\cdots 0 \downarrow 0 \cdots 0 \uparrow 0 \cdots 0 \downarrow 0 \cdots 0 \uparrow 0 \cdots 0 \downarrow 0 \cdots\rangle$$

that is $|\psi_1\rangle(|\psi_2\rangle)$ is the state with hidden antiferromagnetic order where the first non zero spin is $\uparrow(\downarrow)$. Let's recall the mapping[3] (3.11)

$$S_i^z \to \pm\frac{1+\sigma_i^z}{2}\prod_{k<i}(-\sigma_k^z)$$

from which immediately follows

$$(S_i^z)^2 \to \frac{1+\sigma_i^z}{2}$$

We also write down the expressions we found for the string order parameter and the spin-spin correlation functions, eqs. (3.25), (3.12), (3.23) respectively

$$\mathcal{O}_{ij}^z = -\langle\left(\frac{1+\sigma_i^z}{2}\right)\left(\frac{1+\sigma_j^z}{2}\right)\rangle \tag{4.23}$$

[3] The sign is $\pm$ whether the first non zero spin is $\uparrow$ or $\downarrow$

$$\mathcal{C}^z_{ij} = \langle \prod_{k=i}^{j} \sigma^z_k \rangle \tag{4.24}$$

$$\mathcal{C}^x_{ij} = \langle \sigma^x_i \prod_{k=i+1}^{j-1} \left(\frac{1-\sigma^z_k}{2} \right) \sigma^x_j \rangle \tag{4.25}$$

as well as that of the emptiness formation probability (EFP) [90], [67]

$$\mathcal{E}_{ij} = \langle \prod_{k=i}^{j} \left(\frac{1-\sigma^z_k}{2} \right) \rangle \tag{4.26}$$

We can now write down the entries of the density matrix in terms of spin 1/2 operators; it is straightforward for the diagonal elements[4]

-

$$\hat{A}_{11} = \frac{1}{4} \left[\left(\frac{1+\sigma^z_i}{2} \right) \left(\frac{1+\sigma^z_j}{2} \right) - \left(\frac{1+\sigma^z_i}{2} \right) \prod_{k=i+1}^{j-1} (-\sigma^z_k) \left(\frac{1+\sigma^z_j}{2} \right) \right]$$

$$= \frac{1}{4} \left(-\hat{\mathcal{O}}^z_{ij} + (-1)^{j-i} \hat{\mathcal{C}}^z_{ij} \right) \tag{4.27}$$

-

$$\hat{A}_{22} = \frac{1}{2} \left[\left(\frac{1+\sigma^z_i}{2} \right) - \left(\frac{1+\sigma^z_i}{2} \right) \left(\frac{1+\sigma^z_j}{2} \right) \right]$$

$$= \frac{1}{2} \left(\frac{1+\sigma^z_i}{2} + \hat{\mathcal{O}}^z_{ij} \right) \tag{4.28}$$

-

$$\hat{A}_{44} = \frac{1}{4} \left[\left(\frac{1+\sigma^z_i}{2} \right) \left(\frac{1+\sigma^z_j}{2} \right) + \left(\frac{1+\sigma^z_i}{2} \right) \prod_{k=i+1}^{j-1} (-\sigma^z_k) \left(\frac{1+\sigma^z_j}{2} \right) \right]$$

$$= \frac{1}{4} \left(-\hat{\mathcal{O}}^z_{ij} - (-1)^{j-i} \hat{\mathcal{C}}^z_{ij} \right) \tag{4.29}$$

[4]We assume $\prod_{k=i}^{j} \sigma^z_k + \prod_{k=i}^{j-1} \sigma^z_k + \prod_{k=i+1}^{j} \sigma^z_k + \prod_{k=i+1}^{j-1} \sigma^z_k = \mathcal{C}^z_{i,j} + \mathcal{C}^z_{i,j-1} + \mathcal{C}^z_{i+1,j} + \mathcal{C}^z_{i+1,j-1} \simeq \mathcal{C}^z_{i,j}$

- $$\hat{A}_{55} = \left(\frac{1-\sigma_i^z}{2}\right)\left(\frac{1-\sigma_j^z}{2}\right) = -\left(\sigma^z + \hat{\mathcal{O}}_{ij}^z\right) \tag{4.30}$$

We find then, that all the diagonal elements of the two site density matrix can be expressed as linear combinations of the longitudinal string order parameter $\mathcal{O}_z$ and the spin-spin correlation function $\mathcal{C}_z$.

It is now useful to define[5]

$$\hat{\mathcal{P}}_{\{\pm\uparrow i\}} = \frac{1}{2}\left[1 \pm \prod_{k<i}(-\sigma_k^z)\right]\left(\frac{1+\sigma_i^z}{2}\right)$$

$$\hat{\mathcal{P}}_{\{\pm\downarrow i\}} = \frac{1}{2}\left[1 \mp \prod_{k<i}(-\sigma_k^z)\right]\left(\frac{1+\sigma_i^z}{2}\right)$$

i.e. the operators that project on states with a spin $\uparrow(\downarrow)$ on the $i-$th site, and

$$\hat{\mathcal{Q}}_{\{\pm\uparrow i\}} = \frac{1}{2}\left[1 \mp \prod_{k<i}(-\sigma_k^z)\right]$$

$$\hat{\mathcal{Q}}_{\{\pm\downarrow i\}} = \frac{1}{2}\left[1 \pm \prod_{k<i}(-\sigma_k^z)\right]$$

i.e. the operators that ensure that the last non zero spin before site i is $\uparrow(\downarrow)$.

- Let's consider the action of the first term in $\hat{A}_{23}$[6] on $|\Psi\rangle$

  $$\hat{A}_{23}^{(1)}|\Psi\rangle = 0 \ \text{ if} \left[\begin{array}{c} i = \uparrow,\downarrow \\ j = 0,\downarrow \end{array}\right.$$

  So we have a non zero contribution only when $i = 0$ and $j = \uparrow$; in particular, the only case when the hidden order is not broken is when the last non zero spin before i is $\downarrow$ and there is a string of zeroes between i and j

  $$\hat{A}_{23}^{(1)}|\psi_1\rangle = |\cdots 0 \uparrow 0 \cdots 0 \downarrow 0 \cdots 0 \uparrow_i 0 \cdots 0\, 0_j\, 0 \cdots 0 \downarrow 0 \cdots 0 \uparrow 0 \cdots\rangle$$

[5] The sign is $\pm$ whether the first non zero spin is $\uparrow$ or $\downarrow$

[6] We define $\hat{A}_{23}^{(1)} = \frac{1}{2}\langle S_i^z S_i^+ \otimes S_j^- S_j^z\rangle$

and

$$\hat{A}_{23}^{(1)}|\psi_2\rangle = |\cdots 0\downarrow 0\cdots 0\uparrow_i 0\cdots 0\, 0_j\, 0\cdots 0\downarrow 0\cdots 0\uparrow 0\cdots 0\downarrow 0\cdots\rangle$$

We must have then

$$S_i^z S_i^+ \otimes S_j^- S_j^z = \left[\frac{1+\prod_{k<i}(-\sigma_k^z)}{2}\right]\left[\frac{1+\prod_{k<i}(-\sigma_k^z)}{2}\right]\left(\frac{1+\sigma_i^z}{2}\right)\sigma_i^+$$

$$\prod_{k=i+1}^{j-1}\left(\frac{1-\sigma_k^z}{2}\right)\sigma_j^-\left[\frac{1+\prod_{k<j}(-\sigma_k^z)}{2}\right]\left(\frac{1+\sigma_j^z}{2}\right)$$

Taking into account the fact that

$$\left(\frac{1+\sigma_i^z}{2}\right)\sigma_i^+ = \sigma_i^+ \qquad \sigma_j^-\left(\frac{1+\sigma_j^z}{2}\right) = \sigma_j^-$$

we get

$$S_i^z S_i^+ \otimes S_j^- S_j^z = \left[\frac{1+\prod_{k<i}(-\sigma_k^z)}{2}\right]\left[\frac{1+\prod_{k<i}(-\sigma_k^z)}{2}\right]\sigma_i^+$$

$$\prod_{k=i+1}^{j-1}\left(\frac{1-\sigma_k^z}{2}\right)\left[\frac{1+\prod_{k<j}(-\sigma_k^z)}{2}\right]\sigma_j^-$$

Noticing that

$$\prod_{k=i+1}^{j-1}\left(\frac{1-\sigma_k^z}{2}\right)\left[\frac{1+\prod_{k<j}(-\sigma_k^z)}{2}\right] = \left[\frac{1+\prod_{k\leq i}(-\sigma_k^z)}{2}\right]\prod_{k=i+1}^{j-1}\left(\frac{1-\sigma_k^z}{2}\right)$$

and

$$\sigma_i^+\left[\frac{1+\prod_{k<i}(-\sigma_k^z)(-\sigma_i^z)}{2}\right] = \left[\frac{1+\prod_{k<i}(-\sigma_k^z)}{2}\right]\sigma_i^+$$

we finally get

$$S_i^z S_i^+ \otimes S_j^- S_j^z = \left[\frac{1+\prod_{k<i}(-\sigma_k^z)}{2}\right]\left[\frac{1+\prod_{k<i}(-\sigma_k^z)}{2}\right]$$

$$\cdot\left[\frac{1+\prod_{k<i}(-\sigma_k^z)}{2}\right]\sigma_i^+\prod_{k=i+1}^{j-1}\left(\frac{1-\sigma_k^z}{2}\right)\sigma_j^-$$

$$= \left[\frac{1+\prod_{k<i}(-\sigma_k^z)}{2}\right]\sigma_i^+\prod_{k=i+1}^{j-1}\left(\frac{1-\sigma_k^z}{2}\right)\sigma_j^- \tag{4.31}$$

We follow the same steps when we calculate the action of the operator on $|\psi_2\rangle$ keeping in mind that there is a $-$ sign in the projectors. We find

$$S_i^z S_i^+ \otimes S_j^- S_j^z = \left[\frac{1-\prod_{k<i}(-\sigma_k^z)}{2}\right]\sigma_i^+\prod_{k=i+1}^{j-1}\left(\frac{1-\sigma_k^z}{2}\right)\sigma_j^- \tag{4.32}$$

Combining the two terms we have

$$S_i^z S_i^+ \otimes S_j^- S_j^z = \left[\frac{1+\prod_{k<i}(-\sigma_k^z)}{2}\right]\sigma_i^+\prod_{k=i+1}^{j-1}\left(\frac{1-\sigma_k^z}{2}\right)\sigma_j^-$$

$$+\left[\frac{1-\prod_{k<i}(-\sigma_k^z)}{2}\right]\sigma_i^+\prod_{k=i+1}^{j-1}\left(\frac{1-\sigma_k^z}{2}\right)\sigma_j^-$$

$$= \sigma_i^+\prod_{k=i+1}^{j-1}\left(\frac{1-\sigma_k^z}{2}\right)\sigma_j^- \tag{4.33}$$

Proceeding in a completely analogous fashion for $\hat{A}_{23}^{(1)}$ we get

$$\hat{A}_{23} = \hat{\mathcal{P}}_{\{+\uparrow i\}}\sigma_i^+\prod_{k=i+1}^{j-1}\left(\frac{1-\sigma_k^z}{2}\right)\sigma_j^-\hat{\mathcal{P}}_{\{+\uparrow j\}}$$

$$+\hat{\mathcal{P}}_{\{-\uparrow i\}}\sigma_i^+\prod_{k=i+1}^{j-1}\left(\frac{1-\sigma_k^z}{2}\right)\sigma_j^-\hat{\mathcal{P}}_{\{-\uparrow j\}} + h.c.$$

$$= \sigma_i^+\prod_{k=i+1}^{j-1}\left(\frac{1-\sigma_k^z}{2}\right)\sigma_j^- + \sigma_i^-\prod_{k=i+1}^{j-1}\left(\frac{1-\sigma_k^z}{2}\right)\sigma_j^+ = \frac{\hat{\mathcal{C}}_{ij}^x}{2} \tag{4.34}$$

- $$\hat{A}_{45}^\dagger|\psi\rangle = 0 \ \text{ if} \left[\begin{array}{c} i = 0,\downarrow \\ j = \uparrow, 0 \end{array}\right.$$

There is a non zero contribution only when $i = \uparrow$, $j = \downarrow$; in order non to break the hidden order i and j must be between a $\downarrow$ and a $\uparrow$; furthermore we need a string of zeroes between i and j. In the spin 1/2 "language"

$$\hat{A}^{\dagger}_{45} = \sigma_i^- \hat{\mathcal{P}}_{\{+\uparrow i\}} \prod_{k=i+1}^{j-1} \left(\frac{1-\sigma^z_k}{2} \right) \sigma_j^- \hat{\mathcal{P}}_{\{+\downarrow j\}}$$

$$+\sigma_i^- \hat{\mathcal{P}}_{\{-\uparrow i\}} \prod_{k=i+1}^{j-1} \left(\frac{1-\sigma^z_k}{2} \right) \sigma_j^- \hat{\mathcal{P}}_{\{-\downarrow j\}}$$

$$= \sigma_i^- \prod_{k=i+1}^{j-1} \left(\frac{1-\sigma^z_k}{2} \right) \sigma_j^- = \frac{\hat{\mathcal{C}}^x_{ij}}{4} \tag{4.35}$$

-

$$\hat{A}_{46}|\psi\rangle \neq 0 \ \text{ if} \left[\begin{array}{c} i = \downarrow (\uparrow) \\ j = \uparrow (\downarrow) \end{array} \right.$$

The only configuration that gives a non zero contribution and that retains the hidden order is the one with a spin $\downarrow(\uparrow)$ at site i, a spin $\uparrow(\downarrow)$ at site j and spin 0 at all other sites

$$\hat{A}_{46} = \frac{1}{2} \prod_{k<i} \left(\frac{1-\sigma^z_k}{2} \right) \frac{1+\sigma^z_i}{2} \prod_{k=i+1}^{j-1} \left(\frac{1-\sigma^z_k}{2} \right) \hat{\mathcal{P}}_{\{-\uparrow j\}} \prod_{k>j} \left(\frac{1-\sigma^z_k}{2} \right)$$

$$+\frac{1}{2} \prod_{k<i} \left(\frac{1-\sigma^z_k}{2} \right) \frac{1+\sigma^z_i}{2} \prod_{k=i+1}^{j-1} \left(\frac{1-\sigma^z_k}{2} \right) \hat{\mathcal{P}}_{\{+\downarrow j\}} \prod_{k>j} \left(\frac{1-\sigma^z_k}{2} \right)$$

$$= \frac{1}{2} \prod_{k<i} \left(\frac{1-\sigma^z_k}{2} \right) \frac{1+\sigma^z_i}{2} \prod_{k=i+1}^{j-1} \left(\frac{1-\sigma^z_k}{2} \right) \frac{1+\sigma^z_j}{2} \prod_{k>j} \left(\frac{1-\sigma^z_k}{2} \right)$$

$$= \frac{1}{2} \left(\prod_{k} c_k c_k^{\dagger} + \prod_{k \neq i} c_k c_k^{\dagger} + \prod_{k \neq j} c_k c_k^{\dagger} + \prod_{k \neq i,j} c_k c_k^{\dagger} \right) \tag{4.36}$$

and the first term in the last line is an emptiness formation probability(EFP)[7].

Using the expressions obtained, we write down the eigenvalues

$$\lambda_1 = \lambda_2 = \frac{1}{4}\left(-\mathcal{O}^z_{ij} - (-1)^{j-i}\mathcal{C}^z_{ij}\right) \tag{4.37}$$

$$\lambda_{3,4} = \lambda_{5,6} = \frac{1}{2}\left(\frac{1+\langle\sigma^z_i\rangle}{2} + \mathcal{O}^z_{ij}\right) \pm \left|\frac{\mathcal{C}^x_{ij}}{4}\right| \tag{4.38}$$

$$\lambda_{7,8} = \frac{1}{2}\left[\frac{1}{4}\left(-\mathcal{O}^z_{ij} + (-1)^{j-i}\mathcal{C}^z_{ij}\right) + 2\mathcal{E}_{ij} - \left(\langle\sigma^z\rangle + \mathcal{O}^z_{ij}\right)\right.$$

$$\left.\pm\sqrt{\left(\frac{1}{4}\left(-\mathcal{O}^z_{ij} + (-1)^{j-i}\mathcal{C}^z_{ij}\right) + 2\mathcal{E}_{ij} + \left(\langle\sigma^z\rangle + \mathcal{O}^z_{ij}\right)\right)^2 + 2\left(\mathcal{C}^x_{ij}\right)^2}\,\right] \tag{4.39}$$

$$\lambda_9 = \frac{1}{4}\left(-\mathcal{O}^z_{ij} + (-1)^{j-i}\mathcal{C}^z_{ij}\right) + \left(\langle\sigma^z\rangle + \mathcal{O}^z_{ij}\right) \tag{4.40}$$

The isotropic point ($\lambda = 1, D = 0$) is located in the Haldane phase; recalling the asymptotic decay laws for the string order parameters and correlation functions (see subsecs.3.4.1, 3.4.2, 3.4.3, 3.4.4), as well as that for the EFP [67], we get that all the eigenvalues are asymptotically positive, and then the negativity $\mathcal{N}$ is zero, thus according to the Peres-Horodecki criterion [79], [80] the system is not entangled at large distances at the Heisenberg point; it is known [64] that at the isotropic point the negativity of the system is small but non zero, so there must be long distance entanglement [64]. The approximation of our mapping onto the XY model "loses" this feature of the system, thus we conclude that there is entanglement in the spin degrees of freedom and not in the charge ones. . Still, since outside the isotropic point the Peres-Horodecki criterion gives just a necessary condition on the separability of the states, we cannot exclude the presence of *bound* entanglement [81], [82].

[7] We will assume that $A_{46} \simeq 2\mathcal{E}_{ij}$ as $|i-j| \geq 1$, i.e. all the terms in the sum (4.36) give the same contribution, since they can be expressed as pfaffians of matrices which are asymptotycally equivalent

Conclusions

In this thesis we have reconsidered and extended the approach of ref. [59] to the GS properties of spin-1 anisotropic quantum chains. We have included a single-ion term in the Hamiltonian and, moreover, we have analyzed explicitly how the spin-1 correlation functions are written in the spinless fermions language and then in the framework of the XY model in a transverse field for effective spin-1/2 degrees of freedom. In particular, we have focused on the decay laws of the string correlators towards their asymptotic values which apparently were missing in the literature.

The decay laws of string and spin-spin correlation functions (in the longitudinal channel) are all related to the generating function $c(\mathrm{e}^{\mathrm{i}k})$ of equation (3.51) and the determinants of the Toeplitz matrices derived from it. The asymptotic behaviour of the transverse correlation function $\mathcal{C}_x(R)$, instead, originates from a product of two Toeplitz determinants (see the Appendix, in particular eq. (B.2)). The leading terms in the regime $R \gg 1$ for the various correlators are discussed in Sect. 3.4 and summarized in table 3.3. In brief the most interesting points unveiled by the approach used here are:

- The nonvanishing string-order parameters of the spin-1 model (3.2) are simply interpreted as the magnetization along x and z in the XY chain with transverse field (eqs. (3.53) and (3.54)).

- There exists dual behaviour of $\mathcal{O}_x(R)$ and $\mathcal{C}_z(R)$ above and below the transition, both for the asymptotic order parameters and for the decay functional forms.

- The explicit calculation of $\mathcal{C}_x(R)$ allows us to prove an unusual feature in statistical mechanics, already conjectured by Gómez-Santos [59]:

the spin-spin transverse correlation function exhibits always a finite characteristic length Ξ (eq. (3.57)) even when the system becomes critical.

The analytical results are supported by comparison with a numerical (DMRG) study of the model, especially for the correlations $\mathcal{C}_x$ and $\mathcal{O}_z$. A more detailed comparison between the analytical and the numerical estimates should take into account: i) finite-size effects due to a finite total length L while in Sect. 3.2 we passed readily to the thermodynamic limit; ii) corrections for finite distance R beyond the dominant ones. Although in principle they can be computed systematically, in this thesis we have limited ourselves to the leading terms in order to derive analytical expressions with the smallest possible number of fitting parameters.

We studied then the entaglement properties of the model. It is known from the Peres-Horodecki [79], [80] criterion that a mixed state for a bipartite is separable if its partial transpose with respect to one of the two subsystems is positive. Using the symmetries of the λ-D hamiltonian we derived an analytic expression for the negativity $\mathcal{N}$ of the model obtaining essentially the same results as in reference [88]. Using the same approach as in Chapter 3 we have been able to write down all the eigenvalues of the partial transpose of the system in terms of the spin-spin correlators $\mathcal{C}_{x,z}$ (see subsecs. 3.4.2, 3.4.4) and the string correlators $\mathcal{O}_{x,z}$ (see subsecs.3.4.1, 3.4.3,) of the λ-D model, and in the terms of the Emptiness Formation Probability $\mathcal{E}$ of the associated spin 1/2 XY model [67]. We found that at the isotropic Heisenberg point all the eigenvalues are asymptotically (for large separation distances) positive, finding out then $\mathcal{N} \to 0$ asymptotically. According to the Peres-Horodecki criterion we find no entanglement at the Heisenberg point at large distances; it is known [64] that at the isotropic point the negativity of the system is small but non zero, so there must be long distance entanglement [64]. The approximation of our mapping onto the XY model "loses" this feature of the system, thus we conclude that there is entanglement in the spin degrees of freedom and not in the charge ones. Being the criterion only necessary outside the isotropic point, we cannot exclude the presence of *bound* entanglement [81], [82].

Appendix A

Toeplitz forms

In this appendix we shall review the basic definitions and properties of Toeplitz forms and a few theorems we found useful for our purposes. We then give a brief survey on the asymptotic properties of the determinants of Toeplitz matrices. Unless differently cited, the material in the appendix is from the monographs by Böttcher, Grudsky and Silbermann [20], [21], [22].

A.1 Toeplitz matrices: definitions and some useful theorems

An infinite Toeplitz matrix is defined as

$$A = (a_{j-k})_{j,k=0}^{\infty} = \begin{pmatrix} a_0 & a_{-1} & a_{-2} & \cdots \\ a_1 & a_0 & a_{-1} & \cdots \\ a_2 & a_1 & a_0 & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{pmatrix} \tag{A.1}$$

and its large finite section as

$$A = (a_{j-k})_{j,k=0}^{n-1} = \begin{pmatrix} a_0 & \cdots & a_{-(n-1)} \\ \vdots & \ddots & \vdots \\ a_{n-1} & \cdots & a_0 \end{pmatrix} \tag{A.2}$$

The first important result in the theory of Toeplitz forms is the following

Theorem 1 (Toeplitz 1911)**.** *The matrix (A.1) defines a bounded operator on l^2 iff the numbers $\{a_n\}$ are the Fourier coefficients of some function*

$a \in L^\infty(\mathbf{T})$

$$a_n = \frac{1}{2\pi}\int_0^{2\pi} a\left(e^{i\theta}\right)e^{-in\theta}d\theta \qquad\qquad n \in \mathbb{Z} \tag{A.3}$$

In this case the norm of the operator given by (A.1) is

$$\|a\|_\infty = ess\ sup_{t\in\mathbf{T}}\,|a(t)| = inf\{\{c \in \mathbb{R} : \mu\left(\{t : a(t) > c\}\right) = 0\} \tag{A.4}$$

$\mathbf{T}$ being the complex unit circle. If there is a function $a \in L^\infty$ satisfying Th.A.1, this function is unique. In the following we denote both the matrix and the operator it induces on l^2 by $T(a)$, a being defined as the *symbol* of the Toeplitz form.

We cite now the two propositions

Proposition 1 (Gohberg 1952)**.** *The only compact Toeplitz operator is the zero operator.*

Proposition 2. *The Toeplitz operator is self-adjoint if and only if a is real valued.*

Let's now concentrate on continuos symbols. Let $C(T)$ be the set of all continuos functions on the unit circle $\mathbf{T}$. For $a \in L^\infty$, we define the function $\tilde{a} = a(1/t)$ with $t \in \mathbf{T}$. In terms of Fourier series

$$a(t) = \sum_{n=-\infty}^{\infty} a_n t^n \qquad\qquad \tilde{a}(t) = \sum_{n=-\infty}^{\infty} a_{-n} t^n \tag{A.5}$$

and clearly

$$T(a) = \begin{pmatrix} a_0 & a_{-1} & a_{-2} & \cdots \\ a_1 & a_0 & a_{-1} & \cdots \\ a_2 & a_1 & a_0 & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{pmatrix} \qquad T(\tilde{a}) = \begin{pmatrix} a_0 & a_1 & a_2 & \cdots \\ a_{-1} & a_0 & a_1 & \cdots \\ a_{-2} & a_{-1} & a_0 & \cdots \\ \cdots & \cdots & \cdots & \cdots \end{pmatrix} \tag{A.6}$$

and thus $T(\tilde{a})$ is the transpose of $T(a)$. We now define the Hankel operator $H(a)$ generated by the symbol a by the matrix

$$H(a) = (a_{j+k+1})_{j,k=0}^{\infty} = \begin{pmatrix} a_1 & a_2 & a_3 & \cdots \\ a_2 & a_3 & \cdots & \\ a_3 & \cdots & & \\ \cdots & & & \end{pmatrix} \tag{A.7}$$

Proposition 3. *If $a \in C$ then $H(a)$ and $H(\tilde{a})$ are compact operators.*

We have now the following fundamental result on the product of Toeplitz operators

Theorem 2. *If a, $b \in L^\infty$, then*

$$T(a)T(b) = T(ab) - H(a)H(\tilde{b}) \tag{A.8}$$

Theorem 3 (Brown and Halmos 1963 [76])**.** *$T(a)T(b)$ is a Toeplitz operator iff either $a^*(t)$ or $b(t)$ are analytic functions; if the latter condition is satisfied then $T(a)T(b) = T(ab)$.*

Let B be a Banach space and $A \in \mathcal{B}(B)$ with $\mathcal{B}(B)$ a Banach algebra. The operator A is said to be a Fredholm operator if $\mathrm{Im}A$ is a closed subspace of B and the two numbers

$$\alpha(A) = \mathrm{dimKer}A \qquad\qquad \beta(A) = \dim(B/\mathrm{Im}A) \tag{A.9}$$

are finite. If A is Fredholm the index of A is defined as

$$\mathrm{Ind}A = \alpha(A) - \beta(A) \tag{A.10}$$

Theorem 4 (Coburn's Lemma)**.** *Let $a \in L^\infty$ and suppose a does not vanish identically. Then $T(a)$ has a trivial kernel on l^2 or its image is dense in l^2. In particular $T(a)$ is invertible if and only if $T(a)$ is Fredholm of index zero.*

Let's now consider more general matrices of the form

$$A_n = T_n(a) + P_n K P_n + W_n L W_n + C_n \tag{A.11}$$

with $T_n(a)$ the $n \times n$ Toeplitz matrix generated by a, P_n the projection

$$P_n : l^2 \to l^2, \qquad (x_0, x_1, x_2, \cdots) \to (x_0, \cdots, x_{n-1}, 0, 0, \cdots) \tag{A.12}$$

and similarly

$$W_n : l^2 \to l^2, \qquad (x_0, x_1, x_2, \cdots) \to (x_{n-1}, \cdots, x_0, 0, 0, \cdots) \tag{A.13}$$

K and L are compact operators on l^2, and $\{C_n\}$ is a sequence of $n \times n$ matrices such that $\|C_n\| \to 0$.

We have the following results

Proposition 4 (Widom 1976)**.** *If a, $b \in L^\infty$, then*

$$T_n(a)T_n(b) = T_n(ab) - P_n H(a)H(\tilde{b})P_n - W_n H(\tilde{a})H(b)W_n \qquad \text{(A.14)}$$

Theorem 5 (Widom 1976, Silbermann 1981)**.** *Let*[1]

$$\{A_n\} = \{T_n(a) + P_n K P_n + W_n L W_n + C_n\} \in \mathbf{S}(C) \qquad \text{(A.15)}$$

and suppose $T(a) + K$ and $T(\tilde{a}) + L$ are invertible. Then for all sufficiently large n

$$A_n^{-1} = T_n(a^{-1}) + P_n X P_n + W_n Y W_n + D_n \qquad \text{(A.16)}$$

where $\|D_n\| \to 0$ and the compact operators X and Y are given by

$$X = (T(a) + K)^{-1} - T(a^{-1}) \qquad Y = (T(\tilde{a}) + L)^{-1} - T(\tilde{a}^{-1}) \qquad \text{(A.17)}$$

A.2 Asymptotic behavior of Toeplitz determinants

We shall now review the fundamental results on the asymptotic behavior of determinants of Toeplitz matrices[2] generated by the symbol $a(k)$

$$D_n[a] = \det(T_n(a)) = \det\left(\frac{1}{2\pi}\int_{-\pi}^{\pi} dk a(k) e^{-i(j-l)k}\right)_{j,l=0}^{n} \qquad \text{(A.18)}$$

with $a(k)$ a complex periodic function, i.e. $a(k) = a(k + 2\pi)$. In the following we specialize to the asymptotics of determinants of Toeplitz matrices generated by symbols with zero index, the index being defined as

$$\mathrm{Ind}[a(k)] \equiv \frac{1}{2\pi}\int_{-\pi}^{\pi} dk \frac{a'(k)}{(k)} \qquad \text{(A.19)}$$

A.2.1 Strong Szegö limit theorem

Let

$$a(k) = \sum_{m=-\infty}^{\infty} a_m e^{imk} \qquad \text{(A.20)}$$

[1] $\mathbf{S}$ is defined as the set of all sequences $\{A_n\}$ of $n \times n$ matrices such that $\sup_{n\geq 1} \|A_n\| < \infty$

[2] See for instance the recent review [91]

where

$$\sum_{m=-\infty}^{\infty} |a_m| < \infty \qquad\qquad \sum_{m=-\infty}^{\infty} |a_m|^2 m < \infty \tag{A.21}$$

and let

$$a(k) \neq 0 \qquad\qquad \mathrm{Ind}\,[a(k)] = 0 \tag{A.22}$$

Under this assumptions the strong Szegö limit theorem[17], [16] holds, and we have

$$\lim_{n\to\infty} \frac{D_n[a]}{G[a]^{n+1}} = E[a] \tag{A.23}$$

with

$$G[a] = \exp\left(\frac{1}{2\pi}\int_0^{2\pi} dk \ln a(k)\right) \tag{A.24}$$

$$E[a] = \exp\frac{1}{2}\sum_{m=-\infty}^{\infty} \hat{a}_m \hat{a}_{-m}|m| \tag{A.25}$$

In this formula $\hat{a}_m$ is the m-th Fourier coefficient of $\ln a(k)$.

A.2.2 The Fisher-Hartwig conjecture

If the generating function has zeroes, jumps or singularities, Szegö Theorem does not hold anymore, and the Fisher-Hartwig conjecture [18], [93], [96], [97] must be used. Suppose $a(k)$ has R singularities in $k = \theta_r$ ($r = 1, \ldots, R$), we can decompose it as

$$a(k) = \tau(k)\prod_{r=1}^{R} e^{i\kappa_r[(k-\theta_r)\mathrm{mod}\pi-\pi]}\left(2-2\cos(k-\theta_r)\right)^{\lambda_r} \tag{A.26}$$

where $\tau(k)$ is a continuos function satisfying the assumptions of Szegö Theorem. Then according to the Fisher-Hartwig conjecture, the asymptotic behavior of the determinant is given by [18]

$$D_n[a] \sim E[\tau, \{\kappa_j\}, \{\lambda_j\}, \{\theta_j\}] n^{\sum_r (\lambda_r^2-\kappa_r^2)} G[\tau]^n \tag{A.27}$$

with the constant prefactor given by

$$E[\tau, \{\kappa_j\}, \{\lambda_j\}, \{\theta_j\}] \equiv E[\tau]\prod_{r=1}^{R}\left(\tau_-\left(e^{i\theta_r}\right)\right)^{-\kappa_r-\lambda_r}\left(\tau_+\left(e^{-i\theta_r}\right)\right)^{\kappa_r-\lambda_r}$$

$$\prod_{1\le r\neq s\le R}\left(1-e^{i(\theta_s-\theta_r)}\right)^{(\kappa_r+\lambda_r)(\kappa_s-\lambda_s)}\prod_{r=1}^{R}\frac{\mathcal{G}(1+\kappa_r+\lambda_r)\mathcal{G}(1-\kappa_r+\lambda_r)}{\mathcal{G}(1+2\lambda_r)} \tag{A.28}$$

$G[\tau]$ and $E[\tau]$ are defined respectively in (A.24) and (A.25), $\tau_\pm$ are given by the factorization

$$\tau(k)=\tau_-\left(e^{ik}\right)G[\tau]\tau_+\left(e^{-ik}\right) \tag{A.29}$$

such that τ_+ (τ_-) is analytic inside (outside) the unit circle where τ is defined, and satisfies the condition $\tau_+(0)=\tau_-(\infty)=1$. $\mathcal{G}$ is the Barnes G-function, defined by

$$\mathcal{G}(z+1)\equiv(2\pi)^{z/2}e^{-[z+(\gamma+1)z^2]/2}\prod_{n=1}^{\infty}\left(1+\frac{z}{n}\right)^k e^{-z+\frac{z^2}{2n}} \tag{A.30}$$

where $\gamma=0.57721\ldots$ is Euler-Mascheroni constant. The Barnes function satisfies the remarkable identity $\mathcal{G}(z+1)=\Gamma(z)\mathcal{G}(z)$ where $\Gamma(z)$ is the Gamma function.

In general $\tau_\pm$ can be obtained as

$$\ln\tau_+(w)=\frac{1}{2\pi i}\oint dz\frac{\ln\tau(z)}{z-w}\qquad |w|<1$$

$$\ln\tau_-(w)=-\frac{1}{2\pi i}\oint dz\frac{\ln\tau(z)}{z-w}\qquad |w|>1 \tag{A.31}$$

In order to make more evident its analytic structure, we can rewrite the generating function as

$$a(z)=\tau(z)\prod_{r=1}^{R}\left(1-\frac{z}{z_r}\right)^{\lambda_r+\kappa_r}\left(1-\frac{z}{z_r}\right)^{\lambda_r-\kappa_r} \tag{A.32}$$

with $z=e^{ik}$, $z_r=e^{i\theta_r}$.

Fisher-Hartwig conjecture has actually been proven in special cases be several authors [20]: λ,κ real and $|\kappa|<1/2$; $\kappa=0$; $\Re(\kappa)=0$; $\lambda=0$, $|\Re(\kappa)|<1/2$; $\Re(\lambda)\ge0$, $\Re(\kappa)<\Re(\lambda)+1$; $\lambda=0$. $\Re(\kappa)<5/2$; λ,κ complex and $\Re(\lambda)>-1/2$. The conjecture is also proven $\forall\ \lambda,\kappa$ in the case of just one singularity.

A.2.3 Generalized Fisher-Hartwig conjecture

Fisher-Hartwig conjecture must be generalized when more than one inequivalent representations of the generating function in the form (A.26) are possible [96], [97]. In this case the symbol is written as

$$a(k) = \tau^{\imath}(k) \prod_{r=1}^{R} e^{i\kappa_r^{\imath}[(k-\theta_r)\mathrm{mod}2\pi-\pi]} \left(2 - 2\cos(k-\theta_r)\right)^{\lambda_r^{\imath}} \tag{A.33}$$

the index $\imath$ labels the different parametrizations (for $R > 1$ it exists a countable number of parametrizations). The asymptotic formula for the determinant is given by [96], [97]

$$D_n[a] \sim \sum_{\imath\in\Gamma} E[\tau^{\imath}, \{\kappa_a^{\imath}\}, \{\lambda_a^{\imath}\}, \{\theta_a\}] n^{\Omega(\imath)} G[\tau^{\imath}]^n \tag{A.34}$$

with

$$\Omega(\imath) = \sum_r \left((\lambda_r^{\imath})^2 - (\kappa_r^{\imath})^2\right) \tag{A.35}$$

$$\Gamma = \{\imath | \mathrm{Re}[\Omega(\imath)] = \mathrm{max}_j \mathrm{Re}[\Omega(j)]\} \tag{A.36}$$

The generalization of the conjecture gives the asymptotic behavior of the determinant of the Toeplitz matrix as a sum of Fisher-Hartwig-like behaviors calculated for the different inequivalent representations.

A.2.4 Widom's theorem

If $a(k)$ is supported in the interval $\alpha \le k \le 2\pi - \alpha$ Widom's theorem [92] must be applied. In this case the asymptotics of the determinant is given by

$$D_n[a] \sim 2^{1/12} e^{3\zeta'(-1)} \left(\sin\frac{\alpha}{2}\right)^{-1/4} E[\rho]^2 n^{-1/4} G[\rho]^n \left(\cos\frac{\alpha}{2}\right)^{n^2} \tag{A.37}$$

where G e E are defined respectively in (A.24) and (A.25),

$$\rho(k) = a\left(2\cos^{-1}\left[\cos\frac{\alpha}{2}\cos k\right]\right) \tag{A.38}$$

with the convention $0 \le \cos^{-1} x \le \pi$.

A.3 Block Toeplitz matrices

Let $\psi \in L^{\infty}(M)^{N\times N}$ a $n \times n$ matrix valued function defined on the unit circle with Fourier coefficients $\psi_k \in \mathbb{C}^{N\times N}$. Let's consider the set $\mathcal{B}$ made by the functions $\psi \in L^1(M)$ whose Fourier coefficients satisfy

$$\|\psi\|_{\mathcal{B}} := \sum_{k=-\infty}^{\infty} |\psi_k| + \left(\sum_{k=-\infty}^{\infty} |k||\psi_k|^2\right)^{1/2} < \infty \tag{A.39}$$

Endowing the set $\mathcal{B}$ with the above norm, $\mathcal{B}$ becomes a Banach algebra of the continuos functions on the unit circle.

Theorem 6 (Szegö-Widom [95]). *Let $\psi \in \mathcal{B}^{N\times N}$ and suppose that the function $\det\psi$ never vanishes on M and has zero winding number. Then, as $n \to \infty$*

$$\det T_n(\psi) \sim G(\psi)^n E(\psi) \tag{A.40}$$

with

$$G(\psi) = \exp\frac{1}{2\pi}\int_0^{2\pi} \ln\left(\det\psi\left(e^{ix}\right)\right)dx \tag{A.41}$$

and

$$E(\psi) = det\left[T(\psi)T(\psi^{-1})\right] \tag{A.42}$$

We define the Toeplitz operators as

$$T(\psi) = (\psi_{j-k}) \qquad\qquad 0 \le j,k < \infty$$

Unfortunately no explicit expression for $E(\psi)$ is known, unless in some very special cases when further hypothesis are made on the symbol.

Theorem 7 (Widom [94]). *Let $\psi \in \mathcal{B}^{N\times N}$ such that the function $\det\psi$ never vanishes on M and has zero winding number. Suppose $\psi_k = 0\ \forall k > n$ or $\psi_{-k} = 0\ \forall k > n$. Then*

$$E(\psi) = G(\psi)^n \det\left[T_n\left(\psi^{-1}\right)\right] \tag{A.43}$$

Theorem 8 (Widom [94], [68]). *Suppose that, in addition to the conditions of Theorem 6, the matrix ψ^{-1} has the Wiener-Hopf factorization*

$$\psi^{-1}(z) = u_+(z)u_-(z) = v_-(z)v_+(z) \tag{A.44}$$

where the subscribes "+" e "−" indicate analyticity inside and outside of the unit circle, respectively. Suppose also that $\psi(z)$ can be included into a differentiable family $\lambda \to \psi(z,\lambda)$. Then $\ln E(\psi)$ is a differentiable function of λ, and

$$\frac{d}{d\lambda}\ln E(\psi) = \frac{i}{2\pi}\int_{|z|=1} tr\left[\left(u'_+(z)u_-(z) - v'_-(z)v_+(z)\right)\frac{\partial\psi(z,\lambda)}{\partial\lambda}\right]dz \tag{A.45}$$

where ($'$) denotes the derivative with respect to z.

Let's finally consider a generalization of Szegö-Widom theorem [98]. Let $\mathcal{F}$ be the set of all sequences of $n\times n$ matrices $(A_n)_{n=1}^{\infty}$ which are of the form

$$A_n = T_n(a) + P_nKP_n + W_nLW_n + C_n \tag{A.46}$$

with $a \in \mathcal{B}$, K ed L are trace class operators on l^2 and C_n are $n\times n$ matrices that tend to zero in the trace norm. The set of the sequences $(C_n)_{n=1}^{\infty}$ will be denoted by $\mathcal{N}$. Finally P_n e W_n are defined by (A.12) and (A.13). The set $\mathcal{F}$ is a Banach algebra with algebraic operations defined elementwise and the norm

$$\|A_n\|_{\mathcal{F}} = \|a\|_{\mathcal{B}} + \|K\|_1 + \|L\|_1 + \sup_{n\geq 1}\|C_n\|_1 \tag{A.47}$$

where $\|\cdot\|_1$ refers to the trace norm. Let $\mathcal{GB}^{N\times N}$ be the group of all invertible elements in the Banach algebra $\mathcal{B}^{N\times N}$, and denote by $\mathcal{G}_1\mathcal{B}^{N\times N}$ the connected component of $\mathcal{B}^{N\times N}$ containing the identity element.

We are going to consider elements $(A_{n,t})_{n=1}^{\infty} \in \mathcal{F}^{N\times N}$ which depend analytically on a parameter $t \in \Omega$

$$A_{n,t} = T_n(a_t) + P_nK_tP_n + W_nL_tW_n + C_{n,t} \tag{A.48}$$

Theorem 9. *[98] Let Ω be an open subset of $\mathbb{C}$. For each $t \in \Omega$ let $(A_{n,t})_{n=1}^{\infty} \in \mathcal{F}^{N\times N}$, and assume that the map $t \in \Omega \to (A_{n,t})_{n=1}^{\infty} \in \mathcal{F}^{N\times N}$*

is analytic. Moreover, suppose that $a_t \in \mathcal{G}_1\mathcal{B}^{N\times N}$ *where* a_t *generates the Toeplitz matrix* $T_n(a_t)$. *Then* $\forall t \in \Omega$ *the limit*

$$E_t = \lim \frac{A_{n,t}}{G(a_t)^n} \tag{A.49}$$

exists, the convergence is locally uniform on Ω, *and* E_t *depends analytically on* t.

Appendix B

Toeplitz formulation of $\mathcal{C}_x(R)$

The transverse correlation function may be written as (3.23)

$$\mathcal{C}_x = \frac{1}{4}\langle S^+_j S^-_{j+R} + S^-_j S^+_{j+R}\rangle = \langle \sigma^x \prod_{k=j+1}^{j+R-1} \left(\frac{1-\sigma^z_k}{2}\right) \sigma^x_{j+R}\rangle$$

$$= \langle A_j \prod_{k<j} (1-2n_k) \prod_{k=j+1}^{j+R-1} (1-n_k) \prod_{k<j+R} (1-2n_k)\, A_{j+R}\rangle$$

$$= \langle B_j \left(\prod_{k=j+1}^{j+R-1} c_k c^\dagger_k\right) A_{j+R}\rangle = \langle c^\dagger_j \left(\prod_{k=j+1}^{j+R-1} c_k c^\dagger_k\right) c^\dagger_{j+R}\rangle$$

$$+\langle c^\dagger_j \left(\prod_{k=j+1}^{j+R-1} c_k c^\dagger_k\right) c_{j+R}\rangle - \langle c_j \left(\prod_{k=j+1}^{j+R-1} c_k c^\dagger_k\right) c^\dagger_{j+R}\rangle - \langle c_j \left(\prod_{k=j+1}^{j+R-1} c_k c^\dagger_k\right) c_{j+R}\rangle$$

where A and B are defined as usual by

$$A_i = c^\dagger_i + c_i \qquad\qquad B_i = c^\dagger_i - c_i$$

By observing that

$$\langle c^\dagger_j \left(\prod_{k=j+1}^{j+R-1} c_k c^\dagger_k\right) c^\dagger_{j+R}\rangle = \left\langle \left(c^\dagger_j \left(\prod_{k=j+1}^{j+R-1} c_k c^\dagger_k\right) c^\dagger_{j+R}\right)^\dagger \right\rangle$$

$$= -\langle c_j \left(\prod_{k=j+1}^{j+R-1} c_k c^\dagger_k\right) c_{j+R}\rangle$$

$$\langle c_j^\dagger \left(\prod_{k=j+1}^{j+R-1} c_k c_k^\dagger \right) c_{j+R} \rangle = \left\langle \left(c_j^\dagger \left(\prod_{k=j+1}^{j+R-1} c_k c_k^\dagger \right) c_{j+R} \right)^\dagger \right\rangle$$
$$= -\langle c_j \left(\prod_{k=j+1}^{j+R-1} c_k c_k^\dagger \right) c_{j+R}^\dagger \rangle$$

we can write $\mathcal{C}_x(R)$ (using translational and U(1) rotational invariance about z) as

$$\mathcal{C}_x(R) = 2\left[\langle c_j^\dagger \left(\prod_{k=j+1}^{j+R-1} c_k c_k^\dagger \right) c_{j+R}^\dagger \rangle + \langle c_j^\dagger \left(\prod_{k=j+1}^{j+R-1} c_k c_k^\dagger \right) c_{j+R} \rangle \right]$$

Using Wick's theorem [6] we can express the above expectation values as

$$\mathrm{Pf}\left| \begin{array}{cccccccccc}
\mathrm{i}F_1 & \mathrm{i}F_2 & \cdots & \mathrm{i}F_{R-2} & \mathrm{i}F_{R-1} & -H_{-1} & -H_{-2} & \cdots & -H_{-R+1} & -H_{-R} \\
 & \mathrm{i}F_1 & \cdots & \mathrm{i}F_{R-3} & \mathrm{i}F_{R-2} & -H_0 & -H_{-1} & \cdots & -H_{-R+2} & -H_{-R+1} \\
 & & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
 & & & \mathrm{i}F_1 & \mathrm{i}F_2 & -H_{R-4} & -H_{R-5} & \cdots & -H_{-2} & -H_{-3} \\
 & & & & \mathrm{i}F_1 & -H_{R-3} & -H_{R-4} & \cdots & -H_{-1} & -H_{-2} \\
 & & & & & -H_{R-2} & -H_{R-3} & \cdots & -H_0 & -H_{-1} \\
 & & & & & & -\mathrm{i}F_1 & \cdots & -\mathrm{i}F_{R-2} & -\mathrm{i}F_{R-1} \\
 & & & & & & & \ddots & \vdots & \vdots \\
 & & & & & & & & -\mathrm{i}F_1 & -\mathrm{i}F_2 \\
 & & & & & & & & & -\mathrm{i}F_1
\end{array} \right|$$

and

$$\mathrm{Pf}\left| \begin{array}{cccccccccc}
\mathrm{i}F_1 & \mathrm{i}F_2 & \cdots & \mathrm{i}F_{R-2} & \mathrm{i}F_{R-1} & -H_{-1} & -H_{-2} & \cdots & -H_{-R+1} & \mathrm{i}F_R \\
 & \mathrm{i}F_1 & \cdots & \mathrm{i}F_{R-3} & \mathrm{i}F_{R-2} & -H_0 & -H_{-1} & \cdots & -H_{-R+2} & \mathrm{i}F_{R-1} \\
 & & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
 & & & \mathrm{i}F_1 & \mathrm{i}F_2 & -H_{R-4} & -H_{R-5} & \cdots & -H_{-2} & \mathrm{i}F_3 \\
 & & & & \mathrm{i}F_1 & -H_{R-3} & -H_{R-4} & \cdots & -H_{-1} & \mathrm{i}F_2 \\
 & & & & & -H_{R-2} & -H_{R-3} & \cdots & -H_0 & \mathrm{i}F_1 \\
 & & & & & & -\mathrm{i}F_1 & \cdots & -\mathrm{i}F_{R-2} & H_{R-1} \\
 & & & & & & & \ddots & \vdots & \vdots \\
 & & & & & & & & -\mathrm{i}F_1 & H_2 \\
 & & & & & & & & & H_1
\end{array} \right|$$

with

$$F_{l-j} \equiv \mathrm{i}\langle c_j c_l \rangle = -\mathrm{i}\langle c_j^\dagger c_l^\dagger \rangle = \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}k \mathrm{e}^{-\mathrm{i}k(l-j)} f\left(\mathrm{e}^{\mathrm{i}k}\right)$$
$$H_{l-j} \equiv \langle c_j c_l^\dagger \rangle = \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}k \mathrm{e}^{-\mathrm{i}k(l-j)} h\left(\mathrm{e}^{\mathrm{i}k}\right)\mathrm{e}^{-\mathrm{i}k}$$

$$f\left(\mathrm{e}^{\mathrm{i}k}\right) \equiv \frac{\gamma \sin k}{2\sqrt{(\cos k - h)^2 + \gamma^2 \sin^2 k}}\ ,\ \ h\left(\mathrm{e}^{\mathrm{i}k}\right) \equiv \frac{\mathrm{e}^{\mathrm{i}k}}{2}\left(1 + \frac{\cos k - h}{\sqrt{(\cos k - h)^2 + \gamma^2 \sin^2 k}}\right).$$

It is useful to note that $F_{l-j} = -F_{j-l}$ and $H_{l-j} = H_{j-l}$. We now write $\mathcal{C}_x$ as

$$\mathcal{C}_x = -\sqrt{\det \mathbf{M}_1} - \sqrt{\det \mathbf{M}_2} \tag{B.1}$$

where $\mathbf{M}_1$ is a block Toeplitz matrix defined by

$$\mathbf{M}_1 = \begin{pmatrix} -\mathrm{i}\mathbf{F} & -\mathbf{H} \\ \mathbf{H}^{\mathrm{T}} & +\mathrm{i}\mathbf{F} \end{pmatrix} = \mathbf{M}_1[\phi]$$

generated by the matrix-valued symbol (analytically continued to the unit circle)

$$\phi(z) = \begin{pmatrix} -\mathrm{i}f(z) & -h(z) \\ h(z^{-1}) & \mathrm{i}f(z^{-1}) \end{pmatrix}$$

while $\mathbf{M}_2 = \mathbf{M}_1 - \mathbf{M}_0$ with $\mathbf{M}_0$ given by

$$\begin{pmatrix}
0 & \cdots & 0 & 0 & \ldots & 0 & -H_{-R} - \mathrm{i}F_R \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & \ldots & 0 & 0 & \ldots & 0 & -H_{-1} - \mathrm{i}F_1 \\
0 & \cdots & 0 & 0 & \ldots & 0 & -H_{R-1} - \mathrm{i}F_{R-1} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & \ldots & 0 & 0 & \ldots & 0 & -H_1 - \mathrm{i}F_1 \\
H_{-R} + \mathrm{i}F_R & \cdots & H_{-1} + \mathrm{i}F_1 & H_{R-1} + \mathrm{i}F_{R-1} & \ldots & H_1 + \mathrm{i}F_1 & 0
\end{pmatrix}$$

The two matrices $\mathbf{M}_1$ and $\mathbf{M}_2$ are asymptotically equivalent, since their difference $\|\mathbf{M}_0\|_1 \to 0$ as $R \to \infty$ ($\|\cdot\|_1$ being the trace norm); we get then $\det \mathbf{M}_1 = \det \mathbf{M}_2$ so that $\mathcal{C}_x(R) \simeq -2\sqrt{\det \mathbf{M}_1}$. In order to find out the asymptotic behavior of the determinant, we have to study the analytic properties of

$$\det \phi(z) = \frac{1}{2}\left(1 + \mathrm{sign}(z)\frac{z^2 + 1 - 2hz}{\sqrt{\left(z^2 + 1 - 2hz\right)^2 - \gamma^2\left(z^2 - 1\right)^2}}\right);$$

We have, for instance, that when $z = \pm 1$, $\det \phi(\pm 1) = \frac{1}{2}\left(1 + \mathrm{sign}(\pm 1)\mathrm{sign}\left(1 \mp h\right)\right)$ so that for $h < 1$ the symbol is singular at $z = -1$, while for $h > 1$ it is singular at $z = +1$. Unfortunately, as discussed also in [68], [98] known results for the asymptotics of the determinants of Toeplitz matrices generated by matrix-valued symbols do not cover the case of singular symbols with vanishing determinant. Hence, the strategy is to factorize the determinant of $\mathbf{M}_1$ as a product of determinants of matrices generated by scalar-valued symbols. Fortunately, in this case this task is accomplished by transforming $\mathbf{M}_1$ through the matrix

$$\mathbf{U} = \begin{pmatrix} \mathbf{1} & \mathrm{i}\mathbf{F}^{-1}\mathbf{H} \\ \mathbf{0} & \mathbf{1} \end{pmatrix}$$

well defined for even R, so that

$$\mathbf{U}^{\mathrm{T}}\mathbf{M}_1\mathbf{U} = \begin{pmatrix} -\mathrm{i}\mathbf{F} & \mathbf{0} \\ \mathbf{0} & \mathrm{i}\mathbf{F} + \mathrm{i}\mathbf{H}^{\mathrm{T}}\mathbf{F}^{-1}\mathbf{H} \end{pmatrix}. \tag{B.2}$$

Now, we first use a theorem by Widom and Silbermann (see Theorem 5 in Appendix A and, for instance, [20], [21], [22]) according to which $\mathbf{F}^{-1}$ is a Toeplitz matrix generated by f^{-1} (in the present case this result holds for even R) and then express the product $\mathbf{H}^{\mathrm{T}}\mathbf{F}^{-1}\mathbf{H}$ as another Toeplitz matrix generated by the symbol $\mathrm{i}h(z^{-1})f^{-1}(z)h(z)$. The last identification can be done by using repeatedly a theorem by Brown and Halmos (see Theorem 3 [76] in Appendix A):

> *$T(\varphi)T(\psi)$ is a Toeplitz operator iff either $\varphi^*(z)$ or $\psi(z)$ are analytic functions; if the latter condition is satisfied then $T(\varphi)T(\psi) = T(\varphi\psi)$*

where $T(\varphi)$ denotes the Toeplitz matrix generated by the function φ.

We have at last that

$$\det\mathbf{M}_1 = \det\left(-i\mathbf{F}\right)\det\left(i\mathbf{F} + i\mathbf{H}^T\mathbf{F}^{-1}\mathbf{H}\right) \tag{B.3}$$

since $\det\mathbf{U} = 1$.

Let us start by computing $\det(-\mathrm{i}\mathbf{F})$:

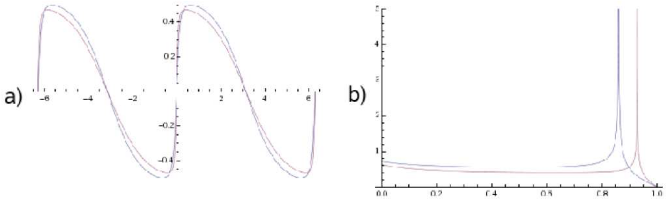

Figure B.1: Plot of the generating function of **F** in the Haldane phase (blue line) and in the Néel phase (red line); in a) it is plotted as a function of k, while in b) we plot its absolute value as a function of $z = e^{ik}$

- *Haldane phase* $h < 1$ ($\lambda_2 > 1$). From the analytic continuation to the unit circle

$$f(z) = -\mathrm{i}\frac{\gamma}{2(1-\gamma)}\mathrm{sign}(z)\frac{(1-z)(1+z)}{\sqrt{(z-\lambda_1)(z-\lambda_2)(1-z\lambda_1)(1-z\lambda_2)}} \tag{B.4}$$

we see that f vanishes at $z = \pm 1$ and is singular at $z = \lambda_{1,2}^{-1}$ (see Figure B.1). This case is covered by the Fisher-Hartwig conjecture (see section A.2.2 and references therein); in order to study the asymptotic behaviour we must find a factorization for the generating function of the form

$$-\mathrm{i}f(z) = \tau(z)\prod_r \left(1 - \frac{z}{z_r}\right)^{\alpha_r+\beta_r}\left(1 - \frac{z_r}{z}\right)^{\alpha_r-\beta_r}$$

where a_r and β_r are defined in table B.1 and the function $\tau(z)$ satisfies the conditions of Szegö's theorem [16]. We find out that

$$\tau(z) = \frac{\gamma}{2(\gamma-1)}\left(-\lambda_1\lambda_2\right)^{-5/4}\left[(z-\lambda_1)(z-\lambda_2)\right]^{-1/2}$$

$$\tau_+ = \left(-\lambda_1\lambda_2\right)^{1/2}\left[(z-\lambda_1)(z-\lambda_2)\right]^{-1/2} \qquad \tau_- = 1$$

We calculate the constants $E[\tau]$ and $G[\tau]$ defined in (A.24), (A.25)

$$G[\tau] = \exp\left(\frac{1}{2\pi}\int_0^{2\pi}\ln\left|\tau(e^{ik})\right|\right) = \frac{\gamma}{2(\gamma-1)}\left(|\lambda_1|\lambda_2\right)^{-7/4} = \exp\left(-\beta_H\right) \tag{B.5}$$

z_r	α_r	β_r
-1	$1/2$	$3/4$
$+1$	$1/2$	$3/4$
λ_1^{-1}	$-1/4$	$-1/2$
λ_2^{-1}	$-1/4$	$-1/2$

Table B.1: Values of z_r, α_r, β_r for the function $f(z)$ (eq. (B.4)) in the Haldane and Néel phases.

$$E[\tau] = \exp\left(\frac{1}{2}\sum_{m=-\infty}^{\infty} \hat{\tau}_m \hat{\tau}_{-m}|m|\right)) = 1 \tag{B.6}$$

The asymptotic behavior turns out to be $\det(-\mathrm{i}\mathbf{F}) \sim E_{\mathrm{H}} R^{-1} \exp(-\beta_{\mathrm{H}} R)$ with the constant prefactor given by

$$E_H = \left[\frac{1+h}{1-h}\right]^{1/2} \left[\frac{\Gamma\left(\frac{5}{4}\right)\Gamma\left(-\frac{1}{4}\right)\Gamma\left(-\frac{3}{4}\right)\Gamma\left(\frac{1}{4}\right)}{\Gamma\left(-\frac{1}{2}\right)}\right]^2$$

$$\cdot \left[\frac{\mathcal{G}\left(\frac{5}{4}\right)\mathcal{G}\left(-\frac{1}{4}\right)\mathcal{G}\left(-\frac{3}{4}\right)\mathcal{G}\left(\frac{1}{4}\right)}{\mathcal{G}\left(-\frac{1}{2}\right)}\right]^2 \tag{B.7}$$

As we have already seen in (A.27) the exponent of the power-law prefactor is given by $\sum_r \left(\alpha_r^2 - \beta_r^2\right)$ where the index r runs over all zero and singular points z_r of $f(z)$

- *Critical line* $h = 1$ ($\lambda_2 = 1$). There is only one zero at $z = -1$ and one singularity at $z = 1/\lambda_1$. The exponents associated with these two points are the same as in the Haldane phase; in this case the power of R receives contributions only from these two points and becomes $[(1/2)^2 - (3/4)^2 + (-1/4)^2 - (-1/2)^2] = -1/2$, instead of -1. However, the characteristic inverse scale in the exponential is nonvanishing even at the critical point

$$\beta_{\mathrm{c}} = \frac{7}{4}\ln|\lambda_1| - \ln\frac{\gamma}{2(\gamma-1)}. \tag{B.8}$$

We calculated the constant prefactor obtaining the same expression as in (B.7) except that the first square bracket is substituted by $\gamma^{-1/4}$ and the powers of the other two square brackets are 1 instead of 2

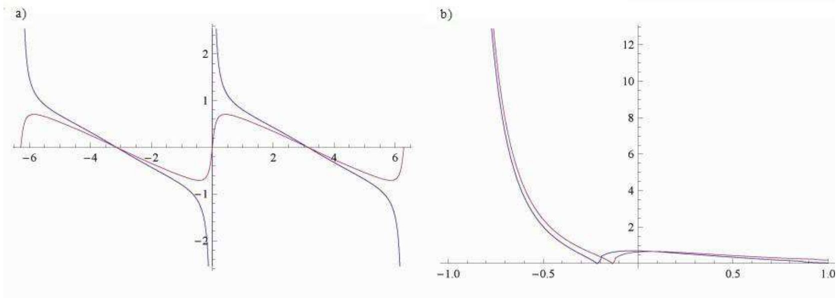

Figure B.2: Plot of the generating function of $\mathbf{G}$ in the Haldane phase (blue line) and in the Néel phase (red line); in a) it is plotted as a function of k, while in b) we plot its absolute value as a function of $z = e^{ik}$

- *Néel phase* $h > 1$ ($\lambda_2 < 1$). The zeroes remain at $z = \pm 1$ while the singularities now are at $z = \lambda_1^{-1}$ and $z = \lambda_2$ (see Fig.B.1). Therefore, we proceed along the same line followed for the Haldane phase, just by replacing $\lambda_2 \leftrightarrow 1/\lambda_2$. In particular, we find the same numbers α_r and β_r as for the case $h < 1$ and thus the asymptotic behaviour remains of the form $\det(-\mathrm{i}\mathbf{F}) \sim E_{\mathrm{N}} R^{-1} \exp(-\beta_{\mathrm{N}} R)$ with

$$\beta_{\mathrm{N}} = \frac{7}{4} \ln \frac{|\lambda_1|}{\lambda_2} - \ln \frac{\gamma}{2(\gamma - 1)}. \tag{B.9}$$

the constant prefactor given by the same expression as (B.7) except for the first term in square brackets given now by $[-(1+h)/(1-h)]^{1/2}$.

Let us now pass to $\det \mathbf{G}$, with $\mathbf{G} = \mathrm{i}\mathbf{F} + \mathrm{i}\mathbf{H}^{\mathrm{T}}\mathbf{F}^{-1}\mathbf{H}$, generated by the symbol (see Figure B.2)

$$g(z) = \mathrm{i}h(z^{-1}) f^{-1}(z) h(z) + \mathrm{i} f(z)$$

$$= -\frac{1}{\gamma} \frac{1}{z^2 - 1} \left[z^2 - 2hz + 1 + z\sqrt{(z + z^{-1} - 2h)^2 - \gamma^2 (z - z^{-1})^2} \right] \tag{B.10}$$

(analytically continued to the unit circle).

- *Haldane phase* $h < 1$ ($\lambda_2 > 1$). The Fisher-Hartwig conjecture (A.2.2) now can be applied, thanks to the following factorization

$$g(z) = \tau(z) (1 - z)^{\alpha_1 + \beta_1} \left(1 - z^{-1}\right)^{\alpha_1 - \beta_1} (1 + z)^{\alpha_2 + \beta_2} \left(1 + z^{-1}\right)^{\alpha_2 - \beta_2} \tag{B.11}$$

z_r	α_r (H)	β_r (H)	α_r (N)	β_r (N)
-1	$1/2$	$1/2$	$1/2$	$1/2$
$+1$	$-1/2$	$-1/2$	$1/2$	$1/2$

Table B.2: Values of z_r, α_r, β_r for the function $g(z)$ in the Haldane and Nel phases.

with $\alpha_{1,2}$ and $\beta_{1,2}$ as in table B.2 and with

$$\tau(z) = \frac{1}{\gamma} \frac{1}{(1+z)^2} \left[z^2 - 2hz + 1 + z\sqrt{\left(z + z^{-1} - 2h\right)^2 - \gamma^2 \left(z - z^{-1}\right)^2} \right]$$

satisfying Szegö's theorem [16]. Consequently, the asymptotic behaviour is purely exponential: $\det \mathbf{G} \sim E'_{\mathrm{H}} \exp(-\beta'_{\mathrm{H}} R)$ where

$$\beta'_{\mathrm{H}} = -\frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}k \ln \left| \cos k - h + \sqrt{(\cos k - h)^2 + (\gamma \sin k)^2} \right| + \ln \frac{\gamma}{2}. \tag{B.12}$$

- *Critical line* $h = 1$ ($\lambda_2 = 1$). There are no singularities and a simple zero at $z = -1$, with exponents α and β as in the first row of table B.2. Therefore, the net power of R in the algebraic prefactor vanishes and the decay is purely exponential with

$$\beta'_{\mathrm{c}} = -\frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}k \ln \left| \cos k - 1 + \sqrt{(\cos k - 1)^2 + (\gamma \sin k)^2} \right| + \ln \frac{\gamma}{2}. \tag{B.13}$$

  As a function of γ, β'_{c} is decreasing for $\gamma > 1$ but does not vanish.

- *Néel phase* $h > 1$ ($\lambda_2 < 1$). With respect to the Haldane phase, the function $\tau(z)$ changes to

$$\tau(z) = \frac{1}{\gamma} \frac{1}{(1+z)^2 (1-z)^2}$$

$$\cdot \left[z^2 - 2hz + 1 + z\sqrt{\left(z + z^{-1} - 2h\right)^2 - \gamma^2 \left(z - z^{-1}\right)^2} \right] \tag{B.14}$$

  while the exponents $\alpha_{1,2}$ and $\beta_{1,2}$ are reported in the fourth and fifth column of table B.2. Again, there is no algebraic prefactor and the constant of the exponential decay, $\det \mathbf{G} \sim E'_{\mathrm{N}} \exp(-\beta'_{\mathrm{N}} R)$, reads

$$\beta'_{\mathrm{N}} = -\frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}k \ln \left| \cos k - h + \sqrt{(\cos k - h)^2 + (\gamma \sin k)^2} \right| + \ln \frac{\gamma}{2} = \beta'_{\mathrm{H}}(\gamma, h). \tag{B.15}$$

Unfortunately we have not been able to evaluate analytically the previous integrals.

Bibliography

[1] E.Ising *Beitrag zür Theorie des Ferromagnetismus* Z.Physik **31** 253 (1925)

[2] E.Lieb, T.Schultz, D.Mattis *Two Soluble models of an Antiferromagnetic Chain* Ann. Phys. **16**, 407 (1961)

[3] I.Affleck, E.Lieb *A Proof of Part of Haldane's Conjecture on Spin Chains* **12** 57 (1986)

[4] S.Katsura *Statistical Mechanics of the Anisotropic Linear Heisenberg Model* Phys.Rev **127**, 1508 (1962)

[5] P.Jordan, E.Wigner Z.Physik **47**, 631 (1928)

[6] E.Caianiello, M.Fubini *On the Algorithm of Dirac Spurs* Nuovo Cimento **9**, 1218 (1952)

[7] S.Sachdev *Quantum Phase Transitions* Cambridge, Cambridge University Press, 1999

[8] T.T.Wu *Theory of Toeplitz Determinants and the Spin Correlations of the Two Dimensional Ising Model.I* Phys.Rev **149**, 380 (1966)

[9] B.McCoy *Spin Correlation Functions of the XY Model* Phys.Rev **173**, 531 (1968)

[10] E.Barouch, B.McCoy, M.Dresden *Statistical Mechanics of the XY Model.I* Phys.Rev.A **2**, 1075 (1970)

[11] E.Barouch, B.McCoy *Statistical Mechanics of the XY Model.II. Spin Correlation Functions* Phys.Rev.A **3**, 786 (1971)

[12] E.Barouch, B.McCoy *Statistical Mechanics of the XY Model. III* Phys.Rev.A **3** 2137 (1971)

[13] B.McCoy, E.Barouch, D.B.Abraham *Statistical Mechanics of the XY Model. IV. Time Dependent Spin Correlation Functions* Phys.Rev.A **4** 2331 (1971)

[14] G.Muller, R.Shrock *Implications of direct-product ground states in the one-dimensional quantum XYZ and XY spin chains* Phys.Rev.B **32**, 5845 (1985)

[15] R.Vein, P.Dale *Determinants and their Application in Mathematical Physics* Springer-Verlag, 1999

[16] I.I.Hirschman *The Strong Szëgo Limit Theorem for Toeplitz Determinants* Amer.J.Math. **88**, 577 (1966)

[17] U.Grenander, G.Szegö *Toeplitz forms and their applications*, University of California Press, 1958

[18] R.E.Hartwig, M.E.Fisher *Asymptotic Behavior of Toeplitz Matrices and Determinants*, Arch.Rational.Mech.Anal. **32** 190, 1969

[19] J.W.L.Glaisher *Note on a relation connecting constants analogous to Euler's constant* Messenger Math. **24** 1 (1894)

[20] A.Böttcher, B.Silbermann *Introduction to Large Truncated Toeplitz Matrices* Springer Verlag 1998

[21] A.Böttcher, S.Grudsky *Toeplitz Matrices, Asymptotic Linear Algebra and Functional Analysis*, Birkhauser 2000

[22] A.Böttcher, B.Silbermann *Analysis of Toeplitz Operators* 2 ed. Springer 2006

[23] H.A.Kramers, G.H.Wannier *Statistics of the Two-Dimensional Ferromagnet. Part I* Phys.Rev. **60** 252, 1941

[24] R.Savit *Duality in Field Theory and Statistical Systems* Rev.Mod.Phys. **52** 453, 1980

[25] H.Hinrichsen, V.Rittenberg *A two-parameter deformation of the SU (1/1) superalgebra and the XY quantum chain in a magnetic field*, Phys.Lett.B **275** 350, 1992

[26] H Hinrichsen *A generalized duality transformation of the anisotropic XY chain in a magnetic field*, J.Phys.A **27** 1121, 1994

[27] H.Bethe *Zür Theorie der Metalle I. Eigenwerte und Eigenfunktionen Atomkete* Zeitschrift für Physik **71**, 205 (1931)

[28] J.des Cloizeaux, J.J.Pearson *Spin-Wave Spectrum of the Antiferromagnetic Linear Chain* Phys. Rev. **128**, 2131 (1962)

[29] N.D.Mermin, H.Wagner *Absence of Ferromagnetism or Antiferromagnetism in One- or Two-Dimensional Isotropic Heisenberg Models* Phys. Rev. Lett. **17**, 1133 (1966)

[30] I.Affleck *Field Theory Methods and Quantum Critical Phenomena* in *Strings,Fields and Critical Phenomena* Les Houches 1988, Session XLIX, E.Brezin, J.Zinn-Justin eds., North-Holland, 1990

[31] A.Auerbach *Interacting Electrons and Quantum Magnetism* Berlin, Springer 1998

[32] E.Fradkin *Field Theories of Condesed Matter Systems* Perseus Books,1998

[33] F.D.Haldane *Nonlinear Field Theory of Large-Spin Heisenberg Antiferromagnets: Semiclassically Quantized Solitons of the One-Dimensional Easy-Axis Nel State* Phys.Rev.Lett. **50**, 1153 (1983)

[34] F.D.Haldane *Continuum Dynamics of the 1-D Heisenberg Antiferromagnet: Identification with the $O(3)$ nonlinear σ model* Phys.Lett. **93A**, 464 (1983)

[35] I.Affleck *Quantum Spin Chains and the Haldane Gap* J.Phys.:Cond.Matter **1**. 3047 (1989)

[36] L.A.Takhtajan *The picture of low-lying excitations in the isotropic Heisenberg chain of arbitrary spins* Phys.Lett. **87A**, 479 (1982)

[37] H.M.Babujian *Exact solution of the one-dimensional isotropic Heisenberg chain with arbitrary spins S* Phys.Lett. **90A**, 479 (1982)

[38] M.den Nijs, K.Rommelse *Preroughening Transitions in Crystal Surfaces and Valence-bond Phases in Quantum Spin Chains* Phys.Rev.B **40**, 4709 (1989)

[39] K.Rommelse, M.den Nijs *Preroughening Transitions in Surfaces* Phys.Rev.Lett. **59**, 2578 (1987)

[40] T.Kennedy, H.Tasaki *Hidden $Z_2 \times Z_2$ Symmetry Breaking in Haldane-gap Antiferromagnets* Phys.Rev.B **45**, 304 (1992)

[41] T.Kennedy, H.Tasaki *Hidden Symmetry Breaking and the Haldane Phase in $S = 1$ Quantum Spin Chains* Comm.Math.Phys. **147**, 431 (1992)

[42] I.Affleck, T.Kennedy, E.H.Lieb, H.Tasaki *Rigorous Results on Valence-bond Ground States in Antiferromagnets* Phys.Rev.Lett. **59**, 799 (1987)

[43] I.Affleck, T.Kennedy, E.H.Lieb, H.Tasaki *Valence Bond Ground States in Isotropic Quantum Antiferromagnets* Comm.Math.Phys. **115**, 477 (1988)

[44] D.P.Arovas, A.Auerbach, F.D.Haldane *Extended Heisenberg Models of Antiferromagnetism: Analogies to the Fractional Quantum Hall Effect* Phys.Rev.Lett. **60**, 531 (1988)

[45] G.Morandi *The Role of Topology in Classical and Quantum Physics* Berlin, Springer 1992

[46] K.G.Wilson, J.B.Kogut *The Renormalization Group and the ϵ Expansion* Physics Reports **12**, 74 (1974)

[47] A.Polyakov *Interaction of Goldstone Particles in two Dimensions. Applications to Ferromagnets and Massive Yang-Mills Fields* Phys.Lett. **59B**, 79 (1975)

[48] H.Tasaki *Quantum liquid in antiferromagnetic chains: a stochastic geometric approach to the Haldane gap* Phys. Rev. Lett. **66** 798, 1991

[49] N.Elstner, H.-J. Mikeska *String correlations of the antiferromagnetic spin-1 chain: Excited states and magnetic field effects* Phys. Rev. B **50** 3907, 1994

[50] A.O.Gogolin, A.A.Nersesyan, A.M.Tsvelik *Bosonization and strongly correlated systems* Cambridge University Press, 1998

[51] L.Campos Venuti, C.Degli Esposti Boschi, E.Ercolessi, G.Morandi, F.Ortolani, S.Pasini, M.Roncaglia *Stable particles in anisotropic spin-1 chains* Eur. Phys. J. B **53** 11, 2006

[52] S.R.White, D.A.Huse. *Numerical renormalization-group study of low-lying eigenstates of the antiferromagnetic* $s = 1$ *Heisenberg chain* Phys. Rev. B **48** 3844, 1993

[53] S.Qin, J.Lou, L.Sun, C.Chen *Nonlocal topological order in antiferromagnetic Heisenberg chains* Phys. Rev. Lett. **90** 067202, 2003

[54] W.Chen, K.Hida, B.C.Sanctuary *Ground-state phase diagram of* $s = 1$ *XXZ chains with uniaxial single-ion-type anisotropy* Phys. Rev. B **67** 104401, 2003

[55] M.T.Batchelor, X.-W.Guan, N.Oelkers *Thermal and magnetic properties of spin-1 magnetic chain compounds with large single-ion and in-plane anisotropies* Phys. Rev. B **70** 184408, 2004

[56] M.Henkel. *Conformal invariance and critical phenomena* Springer, 1999

[57] F.C.Alcaraz, Y.Hatsugai. *String correlation functions in the anisotropic spin-1 Heisenberg chain* Phys. Rev. B **46** 13914, 1992

[58] C.Degli Esposti Boschi, E.Ercolessi, F.Ortolani, M.Roncaglia *On* $c = 1$ *critical phases in anisotropic spin-1 chains* Eur. Phys. J B **35** 465, 2003

[59] G.Gómez-Santos *Variational approach to the XXZ spin-1 linear chain: Elementary excitations and Haldane conjecture* Phys. Rev. Lett. **63** 790, 1989

[60] C.Degli Esposti Boschi, M.Di Dio, G.Morandi, M.Roncaglia *Effective Mapping of Spin-1 Chains onto Integrable Fermionic Models. A Study of String and Néel Correlation Functions* J.Phys.A:Math.Theor. **42** 055002 (2009)

[61] C.Degli Esposti Boschi, F.Ortolani *Investigation of quantum phase transition with multi-target DMRG methods* Eur. Phys. J. B **41** 503, 2004

[62] A.M.Tsvelik *Field-theory treatment of the Heisenberg spin-1 chain* Phys. Rev. B **42** 10499, 1990

[63] A.G.Shelton, A.A.Nersesyan, A.M.Tsvelik *Antiferromagnetic spin ladders: Crossover between spin $s = 1/2$ and $s = 1$ chains* Phys. Rev. B **53** 8521, 1996

[64] L.Campos Venuti, C.Degli Esposti Boschi, M.Roncaglia *Long-distance entanglement in spin systems* Phys. Rev. Lett. **96** 247206, 2006

[65] A.Osterloh, L.Amico, G.Falci, R.Fazio *Scaling of entanglement close to a quantum phase transition* Nature **416** 608, 2002

[66] D.M.Greenberger, M.A.Horne, A.Zeilinger. In M Kafatos, editor, *Bell's theorem, quantum theory, and conceptions of the universe* Kluwer Academic, Dordrecht, 1989

[67] F.Franchini, A.G.Abanov *Aymptotics of Toeplitz determinants and the emptiness formation probability for the XY spin chain* J. Phys. A: Math. Gen. **38** 5069, 2005 Corrigendum in *ibid.* **39** 14533 (2006).

[68] A.R.Its, B.-Q.Jin, V.E.Korepin *Entropy of XY Spin Chain and Block Toeplitz Determinants* in *Universality and Renormalization: From Stochasti Evolution to Renormalization of Quantum Fields*, I.Bender, D.Kreimer (eds) Fields Institute Communications **50**, 151 (2007)

[69] L.Campos Venuti, E.Ercolessi, G.Morandi, P.Pieri, M.Roncaglia *Heisenberg integer spin chains in a uniform magnetic field* Int. J. Mod. Phys. B **16** 1363, 2002

[70] J.Lou, X.Dai, S.Qin, Z.Su, L.Yu *Heisenberg spin-1 chain in a staggered magnetic field: A density-matrix-renormalization-group study* Phys. Rev. B **60** 52, 1999

[71] E.Ercolessi, G.Morandi, P.Pieri, M.Roncaglia *Spin-1 antiferromagnetic Heisenberg chains in an external staggered field* Phys. Rev. B **62** 14860, 2000

[72] T.T.Wu, B.McCoy, C.Tracy, E.Barouch *Spin-Spin Correlation Functions for the Two Dimensional Ising Model: Exact Theory in the Scaling Region* Phys.Rev.B **13**, 316 (1976)

[73] C.K.Lai *Lattice Gas with Nearest-Neighbor Interaction in One Dimension with Arbitrary Statistics* J.Math.Phys. **15**, 1675 (1974)

[74] B.Sutherland *Model for a Multicomponent Quantum System* **12**, 3795 (1975)

[75] W.J.Camp *Decay of order in classical many-body systems. ii. Ising model at high temperatures* Phys. Rev. B **6** 960, 1972

[76] A.Brown, P.R.Halmos *Algebraic Properties of Toeplitz Operators* J.Reine Angew.Math **231**, 89 (1963)

[77] A.Peres *Quantum Theory: Concepts and Methods* Kluwer, Dordrecht (1993)

[78] L.Amico, R.Fazio, A.Osterloh, V.Vedral *Entanglement in Many-Body Systems* Rev.Mod.Phys. **80** 517 (2008)

[79] A.Peres *Separability Criterion for Density Matrices* Phys.Rev.Lett. **77** 1413 (1996)

[80] M.Horodecki, P.Horodecki, R.Horodecki *Separability of Mixed States: Necessary and Sufficient conditions* Phys.Lett.A **223** 1 (1996)

[81] P.Horodecki *Separability Criterion and Inseparable Mixed States with Positive Partial Transposition* Phys.Lett.A **232** 333 (1997)

[82] M.Horodecki, P.Horodecki, R.Horodecki *Mixed-State Entanglement and Distillation: Is There a "Bound" Entanglement in Nature?* Phys.Rev.Lett. **80** 5239 (1998)

[83] K.G.H.Vollbrecht, R.F.Werner *Entanglement Measures under Symmetry* Phys.Rev.A **64** 062307 (2001)

[84] J.Schliemann *Entanglement in $SU(2)$-invariant Quantum Spin Chains* Phys.Rev.A **68** 012309 (2003)

[85] J.Schliemann *Entanglement in $SU(2)$-invariant Quantum Systems: The Positive Partial Transpose Criterion and Others* Phys.Rev.A **72** 012307 (2005)

[86] H.-P.Breuer *Entanglement in $SO(3)$-invariant Bipartite Quantum Systems* Phys.Rev.A **71** 062330 (2005)

[87] H.-P.Breuer *State Space Structure and Entanglement of Rotationally invariant Spin Systems* J.Phys.A:Math.Gen. **38** 9019 (2005)

[88] X.Wang, S.-J.Gu *Negativity, Entanglement Witness and Quantum Phase Transition in Spin-1 Heisenberg Chains* J.Phys.A:Math.Gen. **40** 10759 (2007)

[89] G.Vidal, R.F.Werner *Computable Measure of Entanglement* Phys.Rev.A **65** 032314 (2002)

[90] V.E.Korepin, A.G.Izergin, F.H.L.Essler, D.B.Uglov *Correlation Function of the spin-$\frac{1}{2}$ XXX Antiferromagnet* Phys.Lett.A **190** 182 (1994)

[91] T.Ehrhardt *The Strong Szëgo Limit Theorem for Toeplitz Determinants* Operator Th.: Advances and App. **124**, 217 (2001)

[92] H.Widom *The Strong Szegö Limit Theorem for Circular Arcs* Ind.Univ.Math.J. **21**, 277 (1971)

[93] H.Widom *Toeplitz Determinants with Singular Generating Functions* Amer.J.Math. **95**, 333 (1973)

[94] H.Widom *Asymptotic behavior of block Toeplitz matrices and determinants* Adv. in Math. **13**, 284 (1974)

[95] H.Widom *Asymptotic behavior of block Toeplitz matrices and determinants. II* Adv. in Math. **21**, 1 (1976)

[96] E.L.Basor, C.A.Tracy *The Fisher-Hartwig Conjecture and Generalizations* Physica A **177**, 167 (1991)

[97] E.L.Basor, K.E.Morrison *The Fisher-Hartwig Conjecture and Toeplitz Eigenvalues* Lin.Alg.App. **202**, 129 (1994)

[98] E.L.Basor, T.Ehrhardt *Asymptotics of Block Toeplitz Determinants and the Classical Dimer Model* Commun.Math.Phys. **274**, 427 (2007)